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Integrability, chaos and entanglement in quantum systems

Supervisores: Federico Finkel Morgenstern y Artemio González López

**Asier López Gordón**

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# Study of the Entanglement Entropy of the XX Model

Asier López Gordón[1,*]

[1] *Trabajo de Fin de Grado, Departamento de Física Teórica, UCM*
*Supervisors: Federico Finkel and Artemio González-López*

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We analyse the exact expression and asymptotic behaviour of the entanglement entropy of some integrable spin chains. Our calculations are explicitly carried out for the XX chain, although most of them will be generalizable to other free fermion or equivalent systems. We start by introducing the von Neumann entanglement entropy as a measure of the degree of entanglement between a block of spins and the rest of a spin chain. We present the XX chain and its equivalence to a free fermion system via a Jordan-Wigner transformation of its Hamiltonian. Making use of the translational invariance of the chain, we diagonalise the resulting Hamiltonian through a Fourier transform. From this diagonalised Hamiltonian and inverting the Fourier transform we obtain the correlation matrix of the model. We show a correspondence between the eigenvalues of the correlation matrix and the ones of the density matrix of the system, and exploit this fact to obtain an exact expression for the entanglement entropy. We then consider the scaling of the entanglement entropy of the block when its size grows, as well as the dependence of the criticality of the model with the value of the external magnetic field applied. Moreover, we discuss the relation of entropy scaling and criticality with conformal field theories. We finally obtain explicitly the asymptotic expression of the entanglement entropy of the XX model by making use of a proven case of the Fisher-Hartwig conjecture for Toeplitz matrices.

Analizamos la expresión exacta y el comportamiento asintótico de la entropía de entrelazamiento de algunas cadenas de espines integrables. Nuestros cálculos se llevan a cabo explícitamente para la cadena XX, aunque la mayoría de ellos serán generalizables a otros sistemas de fermiones libres o equivalentes. Comenzamos introduciendo la entropía de entrelazamiento de von Neumann como medida del grado de entrelazamiento entre un bloque y el resto de una cadena de espines. Presentamos la cadena XX y su equivalencia con un sistema de fermiones libres vía una transformación de Jordan-Wigner de su hamiltoniano. Haciendo uso de la invariancia traslacional de la cadena, diagonalizamos el hamiltoniano resultante mediante una transformada de Fourier. A partir de este hamiltoniano diagonalizado e invirtiendo la transformada de Fourier, obtenemos la matriz de correlación del modelo. Demostramos una correspondencia entre los autovalores de la matriz de correlación y los de la matriz densidad del sistema, y explotamos este hecho para obtener una expresión exacta para la entropía de entrelazamiento. A continuación, consideramos el comportamiento asintótico de la entropía de entrelazamiento de un bloque al aumentar su tamaño, así como la relación entre el comportamiento crítico del modelo y el valor del campo magnético externo aplicado. Finalmente, obtenemos explícitamente la expresión asintótica para la entropía de entrelazamiento del modelo XX haciendo uso de un caso probado de la conjetura de Fisher-Hartwig para las matrices de Toeplitz.

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* asierlop@ucm.es

## I. INTRODUCTION

Classically, if the exact state of a certain physical system is known so is the state of each of its subsystems. On the other hand, the state of a quantum system can be known with surety while the states of its subsystems are uncertain. Namely, the complete system could be in a pure state $\rho = |\psi\rangle\langle\psi|$, and yet be formed by two subsystems with mixed states $\rho_1$ and $\rho_2$. To illustrate this, let us consider a system formed by two qubits, with a state

$$|\psi\rangle = \frac{1}{\sqrt{2}}|1\ 0\rangle + \frac{1}{\sqrt{2}}|0\ 1\rangle\,, \qquad \rho = |\psi\rangle\langle\psi| \quad (1)$$

The density matrix of the first qubit is given by the partial trace of $\rho$ with respect to the second qubit, namely

$$\rho_1 = \mathrm{tr}_2\,\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|\,, \quad (2)$$

where $\mathrm{tr}_2$ is the partial trace over the system of qubit 2. It can be shown [2] that the partial trace is the unique operation such that the expectation value has the property

$$\mathrm{tr}\left((M \otimes \mathbb{1}_B)\ \rho\right) = \mathrm{tr}(M\rho_A) \quad (3)$$

for any observable $M$ on subsystem $A$ of a system $A \cup B$. $\rho_1$ is clearly not a pure state; indeed the first qubit has $1/2$ probability to be in the state $|0\rangle$ or $|1\rangle$ and hence the uncertainty is maximal.

Entanglement is not only interesting as a hallmark of quantum mechanics, it also has a great importance for areas like quantum information theory, quantum many-body physics or even the study of black holes [3]. Therefore, it is of considerable interest to define a quantitative measure of how entangled a system is. That is to say, we need a measure of the degree of entanglement of subsystem $A$ (or $B$) of a system $A\cup B$, when the whole system is in a state (pure or mixed) $\rho$. A widely used measure of entanglement is the entropy of the reduced density matrix $\rho_A = \mathrm{tr}_B\,\rho$ (or $\rho_B = \mathrm{tr}_A\,\rho$), known as the entanglement entropy of $\rho_A$. We shall note that this is an entropy in the sense of information theory, regarding $\rho$ as a probability distribution, not a thermodynamic entropy.

There are several definitions of (information) entropy. For the purposes of this work the von Neumann entropy will be sufficient;

$$S[\rho] = -\,\mathrm{tr}(\rho\log\rho), \quad (4)$$

where we have taken $k_B = 1$.

The von Neumann entropy can be regarded as the limit of the Rényi entropy

$$S_\alpha[\rho] = (1-\alpha)^{-1}\log\left(\mathrm{tr}\,\rho^\alpha\right), \quad \alpha > 0 \quad (5)$$

when $\alpha$ goes to 1. It can also be expressed as the Shannon entropy of the eigenvalues of $\rho$:

$$S[\rho] = -\sum_i \lambda_i \log\lambda_i \quad (6)$$

In this paper we shall be considering $\log x$ as the natural logarithm of $x$ [23].

The entropy of a pure state clearly vanishes, whereas a mixed state has non-zero entropy. Continuing with the previous example, the entropy of each qubit is $S_1 = S_2 = \log 2$. The entanglement entropy is a measure of the lack of information on the the state of a subsystem, even when the state of the whole system is completely known. In contrast to thermodynamic entropy, it does not originate from an incomplete knowledge of the microstates compatible with a given macrostate. In fact, non-zero entanglement entropy can be encountered at zero temperature.

The von Neumann entropy is additive, that is $S(\rho_1\otimes\rho_2) = S(\rho_1) + S(\rho_2)$. Moreover, if a composite system $A\cup B$ is in a pure state, then $S_A = S_B$. In our case, we are interested in the use of entanglement entropy to study the quantum correlations of spin chains. We shall determine the entanglement between a block of $L$ contiguous spins and the rest of the chain in the ground state. This procedure could also be used for an arbitrary excited state (non-zero temperature).

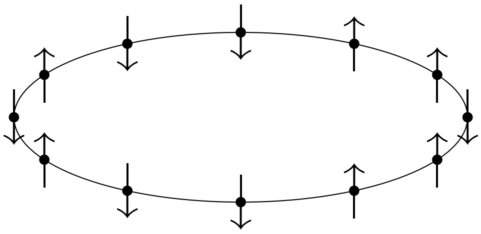

Figure 1. Spin chain with periodic boundary conditions. Each spin site has two possible states: $|\uparrow\rangle$ and $|\downarrow\rangle$.

## II. XX MODEL AND JORDAN-WIGNER TRANSFORMATION

We shall now present a model simple enough to carry out explicit computations while still of interest. The results we are going to obtain will be applicable for a wider family of models, in particular models which are equivalent to a free fermion system.

The XX model is a (one-dimensional) chain of $N$ spin-$\frac{1}{2}$ particles with nearest-neighbour interactions in an external magnetic field, in which spin degrees of freedom are considered (see Fig. 1). This theory can be used as a toy model for the magnetic behaviour of matter, as it captures the structure of a quantum phase transition [4, 5]. In natural units $\hbar = 1$ its Hamiltonian is given by

$$H_{\mathrm{XX}} = \frac{1}{2}\sum_{l=0}^{N-1}\left(\sigma_l^x\sigma_{l+1}^x + \sigma_l^y\sigma_{l+1}^y\right) + \frac{\lambda}{2}\sum_{l=0}^{N-1}\left(\sigma_l^z + 1\right) \tag{7}$$

where $l$ labels the spins, $\lambda$ is the magnetic field and $\sigma_l^x$, $\sigma_l^y$, $\sigma_l^z$ are the Pauli matrices acting on site $l$.

Without loss of generality, we shall consider a magnetic field strenth oriented in the positive $z$-direction, i.e. $\lambda > 0$. If this were not the case we could straightforwardly map the system onto an equivalent one with $\lambda > 0$ by the interchange of up and down spin states. In order to simplify the problem, we are going to assume periodic boundary conditions, in other words, that the sites 0 and $N$ of the chain are the same. Once we consider the thermodynamic limit $N \to \infty$ this election will become irrelevant.

In order to compute the ground state $|\mathrm{GS}\rangle$ of the XX Hamiltonian, we will first perform a Jordan-Wigner transformation to express $H_{\mathrm{XX}}$ as a quadratic form of fermionic operators [1, 5]. This transformation is given by the following relation between the creation and annihilation operators of fermionic modes and the Pauli matrices:

$$a_l = \left(\prod_{m=0}^{l-1}\sigma_m^z\right)\frac{\sigma_l^x - i\sigma_l^y}{2} \equiv \left(\prod_{m=0}^{l-1}\sigma_m^z\right)\sigma_l^- \tag{8}$$

This operators verify the canonical anticommutation relations:

$$\{a_l^\dagger, a_m\} = \delta_{lm} \qquad \{a_l, a_m\} = 0 \tag{9}$$

Without the term in brackets $a_l$ and $a_l^\dagger$ would just be the usual spin ladder operators $\sigma_l^\pm$. Namely, the factor $\sigma_l^-$ corresponds to the operator $|0\rangle_l \langle 1|_l$ in the fermionic occupation basis. The ladder operators verify the same-site anticommutation relations $\{\sigma_l^+, \sigma_l^-\} = 1$. However this equivalence between fermionic operators and spin operators does not work for the many-site problem, as two fermionic operators on different sites anticommute while two spin operators commute ($[\sigma_l^\alpha, \sigma_m^\beta] = 0$ for $l \neq m$). The "string" of operators $\prod_{m=0}^{l-1}\sigma_m^z$ generates the appropriate sign so that the fermionic anticommutation relations are satisfied. Note that the representation of the spin operators in terms of the fermionic operators (or viceversa) is highly non-local.

With our sign election, the fermionic vacuum state $|0\cdots 0\rangle$ is mapped into the state with every spin down in the $z$-direction $|\downarrow\cdots\downarrow\rangle$. Equivalently, we could switch between $a_l$ and $a_l^\dagger$, in which case the vacuum state would map into the state with every spin pointing upwards.

Applying the Jordan-Wigner transformation to the XX Hamiltonian (7) we obtain

$$H_{\mathrm{XX}} = -\sum_{l=0}^{N-1}\left(a_l^\dagger a_{l+1} + a_{l+1}^\dagger a_l\right) + \lambda\sum_{l=0}^{N-1} a_l^\dagger a_l \tag{10}$$

Indeed, we can check that

$$\begin{aligned} a_l^\dagger a_{l+1} = \frac{1}{4}&\sigma_0^z\cdots\sigma_{l-1}^z(\sigma_l^x + i\sigma_l^y) \\ &\times \sigma_0^z\cdots\sigma_{l-1}^z\sigma_l^z(\sigma_{l+1}^x + i\sigma_{l+1}^y) \end{aligned}$$

As Pauli matrices for different sites commute, this can be reordered as

$$a_l^\dagger a_{l+1} = \frac{1}{4}(\sigma_0^z)^2 \cdots (\sigma_{l-1}^z)^2 \\ \times (\sigma_l^x + i\sigma_l^y)\sigma_l^z(\sigma_{l+1}^x - i\sigma_{l+1}^y)$$

Moreover, the Pauli matrices have the following properties:

$$(\sigma^i)^2 = \mathbb{1}, \quad \sigma^i\sigma^j = \delta_{ij}\mathbb{1} + i\varepsilon_{ijk}\sigma^k, \qquad (11)$$

for $i, j, k = x, y, z$, where repeated indices are summed. Therefore the previous expression results in

$$\begin{aligned} a_l^\dagger a_{l+1} =& \frac{1}{4}(-i\sigma_l^y - \sigma_l^x)(\sigma_{l+1}^x - i\sigma_{l+1}^y) \\ =& -\frac{1}{4}(\sigma_l^x\sigma_{l+1}^x + \sigma_l^y\sigma_{l+1}^y) \\ &+ \frac{i}{4}(\sigma_l^x\sigma_{l+1}^y - \sigma_l^y\sigma_{l+1}^x) \end{aligned}$$

whose Hermitian conjugate is

$$\begin{aligned} a_{l+1}^\dagger a_l = \left(a_l^\dagger a_{l+1}\right)^\dagger =& -\frac{1}{4}(\sigma_l^x\sigma_{l+1}^x + \sigma_l^y\sigma_{l+1}^y) \\ &- \frac{i}{4}(\sigma_l^x\sigma_{l+1}^y - \sigma_l^y\sigma_{l+1}^x) \end{aligned}$$

The sum of the two previous expressions gives the first term of the Hamiltonian (7). Analogously, we could verify that

$$a_l^\dagger a_l = \frac{1}{2}\left(\sigma_l^z + \mathbb{1}\right)$$

The operators $a_l^\dagger$ and $a_l$ create and destroy a fermion at site $l$ respectively. Unlike the bosonic case, each site has only two possible states: occupied $|1\rangle_l$ or empty $|0\rangle_l$. The creation operator $a_l^\dagger$ acting over $|1\rangle_l$ thus gives 0. The whole system's Fock space is hence $2^N$-dimensional.

The Hamiltonian (10) corresponds to a system of $N$ spinless fermions [24] attached to the sites of a circular lattice –i.e. the sites 0 and $N$ refer to the same fermion. The terms $a_l^\dagger a_{l+1}$ and $a_{l+1}^\dagger a_l$ correspond to the hopping of a spin between the sites $l$ and $l+1$ –a spin is destroyed at the site $l$ and another one created at the site $l+1$ or the other way around (see Fig. 2). The term $a_l^\dagger a_l$ is the number operator and measures whether the site $l$ is occupied or not. As the

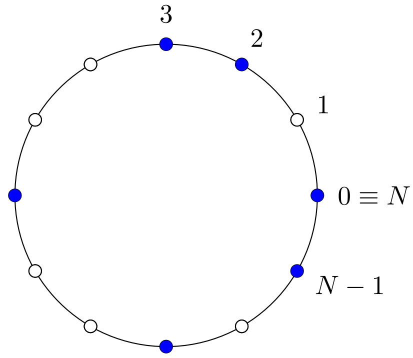


Figure 2. Chain of free fermions with periodic boundary conditions. Each site can be either occupied (by one fermion) or empty, and fermions can hop between adjacent sites.

latter appears as a positive contribution for the Hamiltonian, every site is expected to be empty for high values of $\lambda$. We should note that this Hamiltonian is translationally invariant and that it preserves the total number of fermions.

In general, the Jordan-Wigner transformation maps translationally invariant spin-$\frac{1}{2}$ chains onto free-fermion systems with a Hamiltonian of the form

$$H = \sum_{i \neq j}^{N-1} h_N(i-j) a_i^\dagger a_j, \qquad (12)$$

where $h_N(x) = h_N(-x) = h_N(N-x) \in \mathbb{R}$ is the hopping amplitude.

The translational symmetry motivates the introduction of the Fourier-transformed fermionic operators

$$b_k = \frac{1}{\sqrt{N}} \sum_{l=0}^{N-1} a_l e^{-i\frac{2\pi}{N}kl} \qquad (13)$$

with $0 \le k \le N-1$. Note that the Fourier transform is an unitary transformation, and hence these $b_k$ operators also satisfy the canonical anticommutation relations (9), which means that they are fermionic operators. The translation operator, defined by

$$T\,|s_0 \cdots s_{N-1}\rangle = |s_1 \cdots s_{N-1} s_0\rangle\,, \qquad (14)$$

where $s_l \in \{0, 1\}$ is the occupation number of site $l$, commutes with the Hamiltonian. When $T$ acts on a certain state every spin of the chain gets shifted by one position to the left. With $N$ translations the chain comes back to its original state, i.e. $T^N = \mathbb{1}$, and hence the eigenvalues of $T$ are $e^{2\pi ik/N} \pmod{2\pi}$. The generator of unit translations is the total momentum operator, namely

$$P = -i \log T, \tag{15}$$

which is also conserved. Its eigenvalues are $2\pi k/N \pmod{2\pi}$.

The Hamiltonian (10) (or, more generally, (12)) diagonalises when written in terms of the operators (13), namely

$$H_{\mathrm{XX}} = \sum_{k=0}^{N-1} \Lambda_k b_k^\dagger b_k \equiv \sum_{k=0}^{N-1} \Lambda_k n_k, \tag{16}$$

where $\Lambda_k$ is the energy of the $k$-th mode

$$\Lambda_k = \lambda - 2\cos\left(\frac{2\pi k}{N}\right) \tag{17}$$

(for the Hamiltonian (10)) and $n_k := b_k^\dagger b_k$ is the number operator of mode $k$. The operator $b_k^\dagger$ acting on the vacuum creates a fermion with momentum $2\pi k/N \pmod{2\pi}$ and energy $\Lambda_k$. Indeed, in terms of the occupation numbers basis the action of $b_k^\dagger$ over the vacuum state is

$$b_k^\dagger |0\cdots 0\rangle = \frac{1}{\sqrt{N}}\Big[|1\ 0\cdots 0\rangle + e^{i\frac{2\pi k}{N}}|0\ 1\cdots 0\rangle + \cdots + e^{i\frac{2\pi k}{N}(N-1)}|0\ 0\cdots 1\rangle\Big]$$

and the action of $T$ over that state results in

$$\begin{aligned} T\left(b_k^\dagger |0\cdots 0\rangle\right) =& \frac{1}{\sqrt{N}}\Big[|0\cdots 1\rangle + e^{i\frac{2\pi k}{N}}|1\cdots 0\rangle \\ &+ \cdots + e^{i\frac{2\pi k}{N}(N-1)}|0\cdots 1\ 0\rangle\Big] \\ =& e^{i\frac{2\pi k}{N}} b_k^\dagger |0\cdots 0\rangle, \quad \bmod 2\pi \end{aligned}$$

That is, $b_k^\dagger |0\cdots 0\rangle$ is an eigenstate of $T$ with eigenvalue $e^{2\pi ik/N} \pmod{2\pi}$, and thus it is also an eigenstate of $P$ with eigenvalue $2\pi k/N \pmod{2\pi}$. In particular, the Hamiltonian $H_{\mathrm{XX}}$ and the total momentum $P$ operators are simultaneously diagonalised in the basis of momentum modes.

Note that both positive and negative energy modes are possible. The ground state of the chain is the one in which every negative energy mode is occupied and every positive energy mode is empty. Namely,

$$|\mathrm{GS}\rangle = (b_0^\dagger)^{\varepsilon_0}\cdots(b_{N-1}^\dagger)^{\varepsilon_{N-1}}|0\cdots 0\rangle \tag{18}$$

with

$$\varepsilon_k = \begin{cases} 0 & \text{if } \Lambda_k > 0 \\ 1 & \text{if } \Lambda_k < 0 \end{cases} \tag{19}$$

The ground state energy is thus

$$E(\varepsilon_1,\ldots,\varepsilon_N) = \sum_{k=0}^{N-1} \Lambda_k \varepsilon_k \tag{20}$$

If there were $m$ modes with $\Lambda_k = 0$, the ground state would have $2^m$-fold degeneracy, as the energy of the system would be the same whether they were occupied or unoccupied. In our case $m$ can be at most 2 (for $k \in \{k_c,\ N-k_c\}$), due to the form of the dispersion relation $\Lambda_k$ (see Fig. 3).

If $\lambda > 2$, then $\Lambda_k \geq 0\ \forall\ k$; the external magnetic field dominates and the ground state is simply the vacuum state:

$$|\mathrm{GS}\rangle = |0\cdots 0\rangle, \qquad b_k|\mathrm{GS}\rangle = 0\ \forall\ k, \tag{21}$$

whose energy is 0. Inverting the Fourier and the Jordan-Wigner transformations, we conclude that

$$|\mathrm{GS}\rangle = |{\downarrow}\cdots{\downarrow}\rangle \tag{22}$$

The ground state for high values of the magnetic field is thus, as we expected, a product state and therefore its entanglement entropy is zero.

On the other hand, if $\lambda \in [0, 2)$, in the ground state the modes with $\Lambda_k > 0$ are empty whereas the modes with $\Lambda_k < 0$ are occupied. Hence

$$\begin{aligned} b_k|\mathrm{GS}\rangle = 0 \ \text{ if } \ \Lambda_k > 0 \\ b_k^\dagger|\mathrm{GS}\rangle = 0 \ \text{ if } \ \Lambda_k < 0 \end{aligned} \tag{23}$$

The energy of the ground state in this case is $\sum_k \Lambda_k$ for $k \in [0, k_c] \cup [N-k_c, N-1]$, where

$$k_c = \left[\frac{N}{2\pi}\arccos\left(\frac{\lambda}{2}\right)\right] \tag{24}$$

and $[\cdot]$ denotes the integer part. In the thermodynamic limit, at $\lambda = 2$ (and zero temperature)

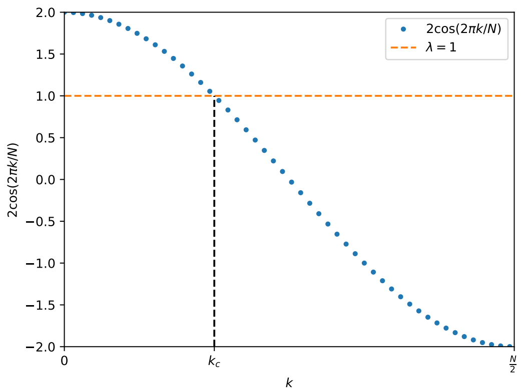


Figure 3. The two contributions to $\Lambda_k$, given by eq. (17), are plotted for the case $\lambda = 1$. The dispersion relation is symmetric with respect to $k = N/2$ ($\Lambda_k = \Lambda_{N-k}$). We observe that $\Lambda_k < 0$ if $2\cos\left(\frac{2\pi k}{N}\right) > \lambda$.

a phase transition occurs [4, 5] from a fully polarized phase ($\lambda > 2$) to a critical phase with quasi-long-range order ($0 \leq \lambda < 2$). The one-way quantum deficit –defined as the difference in the entropy of a subsystem before and after a measurement is performed– can be used as an order parameter, as it vanishes in the polarized phase and is non-zero in the critical one.

We could have applied the Fourier transformation method to any Hamiltonian of the form (12), likewise resulting in a diagonalised Hamiltonian (16) , with $\Lambda_k$ given by the Fourier transform of the hopping amplitude $h_N(x)$ and $k_c$ defined by $\Lambda_k|_{k=k_c} = 0$. This procedure can in fact be extended to a more general type of Hamiltonians:

$$H = H_0 + \sum_{i \neq j} g_{ij} \left( a_i a_j + a_j^\dagger a_i^\dagger \right) \qquad (25)$$

with $H_0$ given by the expression (12), which do not preserve the number of fermions. In this case, exemplified by the XY chain, an additional Bogoliubov transformation [5] is necessary to completely diagonalise the Hamiltonian.

## III. CORRELATION MATRIX METHOD

We are going to compute the von Neumann entanglement entropy of a block of $L$ adjacent spins. As the system has translational symmetry, we can assume they are the first $L$ spins without loss of generality. In order to compute the entropy of the block, we shall follow the method first developed by Vidal, Latorre, Rico and Kitaev [6], based on the correlation matrix $\left\langle a_m^\dagger a_n \right\rangle$ $(0 \leq m, n \leq L-1)$ of the block. From now on we shall assume that expectation values $\langle\, \rangle$ are taken for the ground state of the chain. To begin with, from the equation (23) we can easily obtain the correlation matrix

$$\left\langle b_p^\dagger b_q \right\rangle = \begin{cases} \delta_{pq} & \text{if } \Lambda_p < 0 \\ 0 & \text{if } \Lambda_p > 0 \end{cases}, \qquad (26)$$

where we have considered the orthonormality of the modes in the momentum base. The case $\lambda > 2$ is trivial: as $\left\langle b_p^\dagger b_q \right\rangle$ vanishes, the correlators $\left\langle a_m^\dagger a_n \right\rangle$ are also null. As we already mentioned, the ground state is a product state, and hence its entropy is zero. We shall thus consider the case $0 \leq \lambda < 2$ from now on.

Inverting the Fourier transform we obtain

$$a_n = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{i\frac{2\pi}{N}kn} b_k, \qquad (27)$$

and therefore

$$\begin{aligned} \left\langle a_m^\dagger a_n \right\rangle &= \frac{1}{N} \sum_{k=0}^{N-1} \left\langle b_k^\dagger b_l \right\rangle e^{-i\frac{2\pi}{N}km} e^{i\frac{2\pi}{N}ln} \\ &= \frac{1}{N} \sum_{k=0}^{k_c} \delta_{kl} e^{-i\frac{2\pi}{N}km} e^{i\frac{2\pi}{N}ln} + \frac{1}{N} \sum_{k=k_c+1}^{N-k_c-1} 0 \\ &+ \frac{1}{N} \sum_{k=N-k_c}^{N-1} \delta_{kl} e^{-i\frac{2\pi}{N}km} e^{i\frac{2\pi}{N}ln} \\ = \frac{1}{N} &\left[ \sum_{k=0}^{k_c} e^{-i\frac{2\pi}{N}k(m-n)} + \sum_{k=N-k_c}^{N-1} e^{-i\frac{2\pi}{N}k(m-n)} \right] \end{aligned}$$

Now, the right-hand sum can be rewritten as

$$\begin{aligned}\sum_{k=N-k_c}^{N-1} & e^{-i\frac{2\pi}{N}k(m-n)} \\ &= \sum_{k=N-k_c}^{N} e^{-i\frac{2\pi}{N}k(m-n)} - e^{-i\frac{2\pi}{N}N(m-n)} \\ &= \sum_{k=-k_c}^{0} e^{-i\frac{2\pi}{N}k(m-n)} e^{-i\frac{2\pi}{N}N(m-n)} - 1 \\ &= \sum_{k=0}^{k_c} e^{+i\frac{2\pi}{N}k(m-n)} - 1\end{aligned}$$

Thus the correlation matrix is given by

$$\begin{aligned}\left\langle a_m^\dagger a_n \right\rangle &= \frac{1}{N}\left[\sum_{k=0}^{k_c}\left(e^{-i\frac{2\pi}{N}k(m-n)} + c.c.\right) - 1\right] \\ &= \frac{2}{N}\sum_{k=0}^{k_c}\cos\left[\frac{2\pi}{N}k(m-n)\right] - \frac{1}{N}\end{aligned} \tag{28}$$

Note that so far the only particularity of the XX model we have considered is the value of $k_c$, whereas the form of the correlation matrix (28) is general for any free fermion system. In fact, the method we are going to develop can be applied for a wide family of models. In the thermodynamic limit ($N \to \infty$) the previous sum becomes an integral, which can be determined analytically. In fact, the sum can be computed in closed form even for finite $N$. Let $x = 2\pi k/N$, $\Delta x = 2\pi/N$ and $p_c = 2\pi k_c/N = \arccos(\lambda/2)$. The latter is the so-called Fermi momentum. The correlation matrix of the block of $L$ fermions in position space is then

$$\begin{aligned}A_{mn} \equiv \left\langle a_m^\dagger a_n \right\rangle &= \lim_{\Delta x\to 0}\frac{1}{\pi}\sum_{x=0}^{p_c}\Delta x\cos\left[x\ (m-n)\right] \\ &= \frac{1}{\pi}\int_0^{p_c} \mathrm{d}x\ \cos\left[x\ (m-n)\right] \\ &= \frac{1}{\pi}\frac{\sin\left[p_c(m-n)\right]}{m-n}\end{aligned} \tag{29}$$

with $m,n \in \{0,1,\ldots,L-1\}$. Note that, since $A_{mn}$ depends on $m$ and $n$ through $m-n$ only, we can thus take $m,n \in \{1,\ldots,L\}$, which will slightly simplify the notation. This type of matrices are known as Toeplitz matrices, and we will make use of their properties to determine the asymptotic value of the entropy in the thermodynamic limit (see Section V).

Wick's theorem, extensively used for free particles in quantum field theory, can also be applied to the XX chain fermionic operators. Namely, any operator acting on the block can be expressed in terms of the correlation matrix $A_{mn}$. For instance,

$$\begin{aligned}\left\langle a_k^\dagger a_l^\dagger a_m a_n \right\rangle &= \left\langle \overline{a_k^\dagger a_l^\dagger}\, a_m a_n \right\rangle - \left\langle a_l^\dagger\, \overline{a_k^\dagger a_m}\, a_n \right\rangle \\ &\quad + \left\langle a_l^\dagger a_m\, \overline{a_k^\dagger a_n} \right\rangle \\ &= 0 - \left\langle a_k^\dagger a_m \right\rangle \left\langle a_l^\dagger a_n \right\rangle + \left\langle a_k^\dagger a_n \right\rangle \left\langle a_l^\dagger a_m \right\rangle\end{aligned}$$

where $\overline{AB}$ is the fermionic pairing between operators $A$ and $B$. This is due to the fact that the ground state of the chain is Gaussian with respect to the set of operators $\{a_m,\ a_m^\dagger\}_{0\le m\le N-1}$, that is

$$\left\langle a_m^{(\dagger)} \right\rangle = 0, \quad \overline{a_m^{(\dagger)} a_n^{(\dagger)}} = \left\langle a_m^{(\dagger)} a_n^{(\dagger)} \right\rangle \in \mathbb{C} \tag{30}$$

for all $m,n \in \{0,\ldots,N-1\}$.

On the other hand, the correlation matrix $A_{mn}$ could also be computed through the density matrix as any expectation value:

$$A_{mn} = \mathrm{tr}\left(a_m^\dagger a_n \rho\right) \tag{31}$$

As $a_m^\dagger$ and $a_n$ act on the block of the first $L$ sites only, this must be equal to the partial trace of the reduced density matrix of the block $L$

$$A_{mn} = \mathrm{tr}_L\left(a_m^\dagger a_n \rho_L\right) \tag{32}$$

The correlation matrix $\mathbf{A} \equiv (A_{mn})_{1\le m,n\le L}$ is Hermitian, and hence can be diagonalised via a unitary transformation $\mathbf{U} \equiv (u_{pq})_{1\le p,q\le L}$, that is

$$\mathbf{U}\mathbf{A}\mathbf{U}^\dagger = \mathrm{diag}(\nu_1,\ldots,\nu_L) \equiv \mathbf{G} \tag{33}$$

where $\nu_1,\ldots,\nu_L$ are the eigenvalues of $\mathbf{A}$. Let us introduce the operators

$$g_p = \sum_{m=1}^{L}\overline{u_{pm}}\ a_m \tag{34}$$

where the bar denotes the complex conjugate, which verify the canonical anticommutation relations, since $\mathbf{U}$ is unitary. Their correlation matrix is $\mathbf{G}$, namely

$$\mathrm{tr}_L\left(g_p^\dagger g_q \rho_L\right) = \left\langle g_p^\dagger g_q\right\rangle = \nu_p \delta_{pq} \tag{35}$$

with $1 \leq p, q \leq L$, on account of Eq. (33). The matrix representation of these operators in their computational basis is

$$g_m = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad g_m^\dagger = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \tag{36}$$

Consider now the operators [7]:

$$\begin{aligned} O_p^{(0)} &\equiv g_p^\dagger g_p, \quad O_p^{(1)} \equiv g_p g_p^\dagger \\ O_p^{(2)} &= g_p, \qquad O_p^{(3)} = g_p^\dagger \end{aligned} \tag{37}$$

It is straightforward to check (e.g., making use of the matrix representation) that these operators are orthonormal with respect to the standard Hilbert-Schmidt inner product, that is

$$\mathrm{tr}\left(O_p^{(\alpha)\dagger} O_p^{(\beta)}\right) = \delta_{\alpha\beta} \tag{38}$$

It follows that the operators $\{O_0^{\alpha_1} \cdots O_L^{\alpha_L} : 0 \leq \alpha_i \leq 3\}$ form an orthonormal basis of linear operators $\mathcal{H}_L \to \mathcal{H}_L$, where $\mathcal{H}_L$ is the Hilbert space of the block (and $\mathcal{H}_L \otimes \mathcal{H}_{N-L}$ the Hilbert space of the complete chain). In fact, if we make use of the multiplicative property of the trace with respect to tensor products we get [25]

$$\begin{aligned} &\mathrm{tr}_L\left[\left(O_1^{(\alpha_1)} \cdots O_L^{(\alpha_L)}\right)^\dagger O_1^{(\beta_1)} \cdots O_L^{(\beta_L)}\right] \\ &\quad = \pm\,\mathrm{tr}_L\left[O_1^{(\alpha_1)\dagger} O_1^{(\beta_1)} \cdots O_L^{(\alpha_L)\dagger} O_L^{(\beta_L)}\right] \\ &= \pm \prod_{i=1}^{L} \mathrm{tr}\left(O_i^{\alpha_i \dagger} O_i^{\beta_i}\right) = \delta_{\alpha_1\beta_1} \cdots \delta_{\alpha_L\beta_L} \end{aligned} \tag{39}$$

We can hence write the reduced density matrix of the block at the ground state in terms of this basis:

$$\rho_L = \sum_{1 \leq \alpha_1, \ldots, \alpha_L \leq 3} \rho_L^{\alpha_1 \cdots \alpha_L} \tag{40}$$

with

$$\rho_L^{\alpha_1 \cdots \alpha_L} = \mathrm{tr}_L\left[\left(O_1^{(\alpha_1)} \cdots O_L^{(\alpha_L)}\right)^\dagger \rho_L\right] \tag{41}$$

Since the operators $O_p^{(\alpha_p)}$ (and their adjoints) act only on $\mathcal{H}_L$, we have

$$\begin{aligned} \rho_L^{\alpha_1 \cdots \alpha_L} &= \mathrm{tr}\left[\left(O_1^{(\alpha_1)} \cdots O_L^{(\alpha_L)}\right)^\dagger \rho\right] \\ &\equiv \overline{\left\langle O_1^{(\alpha_1)} \cdots O_L^{(\alpha_L)}\right\rangle}. \end{aligned} \tag{42}$$

It can be shown that the ground state is also Gaussian with respect to the set $\{g_p,\ g_p^\dagger\}_{0 \leq p \leq L-1}$, and thus the matrix elements $\rho_L^{\alpha_1 \cdots \alpha_L}$ are expressible in terms of the second moments of the operators $g_p$ and $g_p^\dagger$. Furthermore, since

$$\langle b_i b_j \rangle = \left\langle b_i^\dagger b_j^\dagger \right\rangle = 0 \tag{43}$$

by linearity we have

$$\langle g_p g_q \rangle = \left\langle g_p^\dagger g_q^\dagger \right\rangle = 0 \tag{44}$$

Additionally, by equation (35) we have

$$\left\langle g_p^\dagger g_q \right\rangle = \nu_p \delta_{pq}, \quad \left\langle g_p g_q^\dagger \right\rangle = (1 - \nu_p)\delta_{pq} \tag{45}$$

From Wick's theorem and equation (42) it then follows that the only matrix elements $\rho_A^{\alpha_1 \cdots \alpha_L}$ that do not vanish are those with $\alpha_p \in \{0, 1\}$ for all $p$. We then have

$$\rho_L^{\alpha_1 \cdots \alpha_L} = \prod_{i=1}^{L} \mu_i(\alpha_i) \tag{46}$$

with $\mu_i(0) = \nu_i$ and $\mu_i(1) = 1 - \nu_i$, and thus

$$\begin{aligned} \rho_L &= \prod_{p=1}^{L} \sum_{\alpha_p \in \{0,1\}} \mu_p(\alpha_p)\, O^{(\alpha_p)} \\ &= \prod_{p=1}^{L} \left[\nu_p g_p^\dagger g_p + (1 - \nu_p) g_p g_p^\dagger\right] \end{aligned} \tag{47}$$

Hence $\rho_L$ is uncorrelated, and can be written as the tensor product:

$$\rho_L \equiv \varrho_1 \otimes \cdots \otimes \varrho_L \tag{48}$$

with $\varrho = \nu_l g_l^\dagger g_l + (1 - \nu_l) g_l g_l^\dagger$. In terms of its matrix representation (in basis of modes of the operators $g_p$ and $g_p^\dagger$)

$$\varrho_p = \begin{pmatrix} \nu_p & \\ & 1 - \nu_p \end{pmatrix}, \tag{49}$$

Since the von Neumann entropy is additive, the entanglement entropy of the block is then, by its its definition (4),

$$S_L = \sum_{l=1}^{L} S[\rho_\ell] = \sum_{l=1}^{L} H_2(\nu_l), \tag{50}$$

where

$$H_2(x) = -x\log x - (1-x)\log(1-x) \tag{51}$$

is the binary entropy.

To sum up, we have obtained an *exact* formula for the entanglement entropy of the ground state of a block of $L$ adjacent spins for the XX model in terms of the eigenvalues $\nu_l$ of its correlation matrix. We should emphasise the computational efficiency of this method, since its computational cost scales polynomially with the number of spins of the block, $\mathcal{O}(L^3)$ [26], whereas the Hilbert space of the block is $2^L$-dimensional.

It is worth noting that there is no need to invert the Jordan-Wigner transformation back to the spin basis. This is due to the fact that the Schmidt coefficients of the ground state are identical when written in terms of the spin basis or in terms of the fermionic creation and annihilation operators. Namely,

$$\begin{aligned} |\mathrm{GS}\rangle &= \sum_{l_0,\ldots,l_{N-1}} C_{l_0,\ldots,l_{N-1}} (a_0^\dagger)^{l_0} \cdots (a_{N-1}^\dagger)^{l_{N-1}} |0\rangle \\ &= \sum_{l_0,\ldots,l_{N-1}} C_{l_0,\ldots,l_{N-1}} |l_0 \cdots l_{N-1}\rangle \,, \end{aligned} \tag{52}$$

where $l_i \in \{0,1\}$ for $i \in \{0,\cdots,N-1\}$, $l_i = 0$ (resp. $l_i = 1$) corresponds to the spin at site $i$ pointing downwards (resp. upwards).

Let us keep in mind that the only particularity of the XX model is still its dispersion relation, more specifically the value of $p_c$. In fact, the correlation matrix method is quite general. It works for any dimension [9], for arbitrary quadratic Hamiltonians and even at finite temperature. It has hence been used in a large number of scenarios, such as homogeneous chains, defect problems or random systems. This approach is equally applicable to coupled oscillators in the ground state.

## IV. SCALING OF ENTANGLEMENT

The procedure explained above provides an effective way for evaluating the entanglement entropy $S_L$ for any fixed $L$. However, Eq. (50) as its stands does not yield itself to the determination of the asymptotic behaviour of $S_L$ as $L \to \infty$, which as we shall see is crucial for ascertaining the criticality properties of the system. This asymptotic behaviour can, however, be determined using a method developed by Jin and Korepin [7], based on the Fisher-Hartwig conjecture for Toeplitz matrices, that we shall outline in the next section. To formulate Jin and Korepin's result we define the scaling variable

$$\mathcal{L} := L\sqrt{1-\left(\frac{\lambda}{2}\right)^2}, \qquad \lambda < 2 \tag{53}$$

in terms of which the entanglement entropy scales as [7]

$$S_L \approx \begin{cases} \frac{\mathcal{L}}{\pi}\log\left(\frac{\pi}{\mathcal{L}}\right), & \text{if } 0 < \mathcal{L} \ll 1 \\ \frac{1}{3}\log(2\mathcal{L}) + \Upsilon_1, & \text{if } \mathcal{L} \gg 1 \end{cases} \tag{54}$$

where $\Upsilon_1$ is a non-universal constant (see next section for more details). First, let us consider a case in which the asymptotic behaviour is particularly easy to determine, namely when $p_c L \ll 1$ and therefore $p_c \ll 1/L \ll 1$. The correlation matrix is given by

$$\begin{aligned} A_{mn} &= \begin{cases} \frac{1}{\pi}\frac{1}{m-n}\left[p_c(m-n) + \mathcal{O}\left(p_c(m-n)\right)^2\right], & m \neq n \\ \frac{p_c}{\pi}, & m = n \end{cases} \\ &\simeq \frac{p_c}{\pi}, \end{aligned} \tag{55}$$

or in matrix form

$$\mathbf{A} \equiv (A_{mn}) \simeq \frac{p_c}{\pi} \begin{pmatrix} 1 & 1 & \cdots & 1 & 1 \\ 1 & 1 & \cdots & 1 & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 1 & \cdots & 1 & 1 \\ 1 & 1 & \cdots & 1 & 1 \end{pmatrix}_{L\times L} . \tag{56}$$

With elementary algebra methods we can obtain the eigenvalues of the matrix above, which turn out to be $\nu = p_c L/\pi$ and $\nu = 0$, with multiplicity

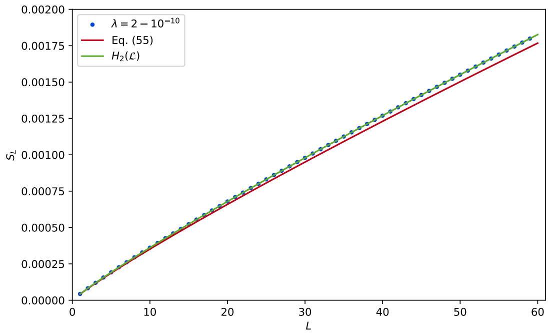


Figure 4. Exact entropy of a block of $L$ spins in the ground state for the XX model with $\lambda = 2 - 10^{-10}$, and fitting to Eq. (54) and to $H_2(\mathcal{L})$.

1 and $L-1$ respectively. The entropy of the block is therefore

$$\begin{aligned} S_L = H_2\left(\frac{p_c L}{\pi}\right) &\simeq -\frac{p_c L}{\pi}\log\left(\frac{p_c L}{\pi}\right) \\ &= \frac{p_c L}{\pi}\log\left(\frac{\pi}{p_c L}\right) \end{aligned} \tag{57}$$

where in the approximation we have again taken into account that $p_c L \ll 1$, and then the second term in Eq. (51) dominates over the first one [27]. This case occurs when the Fermi momentum $p_c$ is given by $p_c = \arccos(\lambda/2) \ll 1$, and thus $\lambda \to 2^-$.

The case above corresponds to equation (54) for $0 < \mathcal{L} \ll 1$. Indeed,

$$\lambda \to 2^- \iff p_c \to 0^+ \Rightarrow \mathcal{L} = L \sin p_c \simeq L p_c$$

In Figure 4 we can see the dependence of $S_L$ on $L$ for $\lambda \to 2^-$, as well as a fitting to the first line in Eq. (54) and to $H_2(\mathcal{L})$.

We are interested in the scaling of the entanglement entropy as the size $L$ of the block of spins we are considering grows. For quantum chains this scaling largely reflects the critical behaviour of the system, and its related behaviour under conformal transformations as we shall now explain. It is widely known that the thermodynamic entropy has an extensive nature, in other words, it shows volume scaling. However, this behaviour is not encountered in the entanglement entropy of typical ground states [3], where an area law, or an area law with a small (frequently logarithmic) correction, appears instead. This roughly means that if a certain region is considered, its entanglement entropy grows proportionally to the size of its boundary.

Area laws are particularly important in one-dimensional systems, where the boundary of a block consist of only two sites for periodic boundary conditions. An area law then implies that the entropy of the chain is upper bounded by a certain constant independent of the block size $L$ and the chain size $N$, i.e. $S(\rho_L) = \mathcal{O}(1)$. Whether this area law holds or not largely depends on the criticality of the system. We say that the system is non-critical whenever the energy gap $\Delta E$ between the ground state and the first excited state satifies $\Delta E \geq c > 0$ as $N \to \infty$, for a certain size-independent constant $c$. The entanglement entropy saturates for a gapped system away from the critical point, and hence an area law holds [28]; whereas when the system is critical the numerical study indicates an unbounded growth of the entropy. More specifically, in fermionic one-dimensional systems (such as the XX chain, via the Jordan-Wigner transformation) $S_L$ is $\mathcal{O}(\log L)$ in the "gapless" (critical) phase and, typically, $\mathcal{O}(1)$ in the "gapped" (non-critical) phase. In the latter case, $S_L$ usually tends to a constant, which is 0 in the model that concerns us. This is again a manifestation of the area law for $d$-dimensional systems, whose respective laws would be $L^{d-1}\log L$ and $L^{d-1}$, $L$ being a characteristic length.

The XX model is critical for $\lambda \leq 2$. Let us recall that we are assuming that $\lambda \geq 0$. For $\lambda > 2$ the dominant term of the Hamiltonian (10) is always positive and proportional to the number operator of fermionic occupation modes, hence there is a non-zero energy gap for every system size and the system is non-critical in this range of $\lambda$. On the contrary, for $\lambda < 2$ the hopping of spins between neighbouring sites dominates. If we look at the energy modes (17) of the Fourier-transformed Hamiltonian (16) we can make certain $\Lambda_k$ arbitrarily close to zero as $N$ becomes larger, and thus the energy gap vanishes ($\Delta E \to 0$ as $N \to \infty$). This illustrates the phase transition that takes place at $\lambda = 2$.

Since a one-dimensional gapless system has no natural scale (which the gap $\Delta E$ would provide, as it has units of length$^{-1}$ for $\hbar = 1$), it is invariant under dilations. Hamiltonians invariant under translations, rotations and scaling transformations usually turn out to have the symmetry of the larger conformal group [10] –the set of transformations that do not change the angles between two arbitrary curves crossing each other at some point. In such a case, the model is equivalent to a certain conformal field theory (CFT) in the low-energy regime. The universality class of these theories (see Appendix A) is the central charge $c$, a parameter that roughly quantifies the "degrees of freedom" of the theory. More specifically, $c$ is an operator that commutes with all the other generators of the Virasoro algebra. Classically the central charge is zero, and it appears quantically as an additive term in the classical commutation relations for the (infinite-dimensional) Virasoro algebra. If a certain one-dimensional system is critical, knowing its universality class (i.e., the $c$ of the effective CFT to which it is equivalent at low energies) is crucial. The asymptotic behaviour of $S_L$ happens to be one of the most powerful tools to determine this parameter. In fact, a necessary (but generally not-sufficient) condition for a system to be critical is that $S_L$ be proportional to $\log L$ as $L \to \infty$ [29]. If this happens, its central charge can be computed by evaluating $\lim_{L\to\infty} S_L/\log L$. This limit can be calculated analytically for the XX model, making use of Eq. (54), namely

$$S_L \simeq \frac{1}{3}\log L + \gamma_1(\lambda), \tag{58}$$

with

$$\gamma_1(\lambda) := \Upsilon_1 + \frac{1}{3}\log\left(2\sin p_c\right) = \Upsilon_1 + \frac{1}{6}\log\left(4-\lambda^2\right) \tag{59}$$

where $\Upsilon_1$ is a constant that was determined analytically by Jin and Korepin.

In Figure 5 we can observe the variation of the entropy with $L$ for different values of the magnetic field. The maximum entropy appears for $\lambda = 0$, when there is no external magnetic field to which spins tend to align. Furthermore, we can see that for both values of $\lambda$ the leading scale of the entropy is perfectly fitted by Eq. (58).

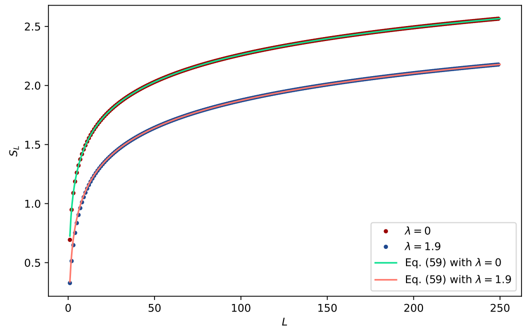


Figure 5. Exact entropy of a block of $L$ spins in the ground state for the XX model and fitting to Eq. (58). Note that the maximal entropy is reached in the absence of external magnetic field ($\lambda = 0$). The entropy decreases with the increase of $\lambda$ until at $\lambda = 2$ a phase transition occurs, the system reaches the ferromagnetic limit, the ground state becomes a product state in the spin basis and $S_L = 0$.

## V. TOEPLITZ DETERMINANT

We shall now make use of the fact that the correlation matrix is a Toeplitz matrix. This type of matrices have been widely studied in mathematics. More specifically, the Fisher-Hartwig conjecture [14], which has been proven for certain cases by Basor [15] and by Böttcher and Silbermann [16], provides the asymptotic behaviour of a Toeplitz matrix determinant when its size goes to infinity. The application of this conjecture (in this case, actually theorem) for the computation of the XX model entanglement entropy in the thermodynamic limit was first proposed by Jin and Korepin in Ref. [7].

Let us recall that a matrix $\mathbf{T}$ is Toeplitz if its elements $T_{ij}$ depend only on $i - j$. Let $c(z)$ be a complex-valued function defined on the unit circle $S^1 = \{z \in \mathbb{C} : |z| = 1\}$. Then its Fourier coefficients $c_n$ ($n \in \mathbb{Z}$) are defined by

$$\begin{aligned} c_n &= \frac{1}{2\pi i}\int_{|z|=1} c(z) z^{-n-1}\mathrm{d}z \\ &\equiv \frac{1}{2\pi}\int_0^{2\pi} c\left(e^{i\theta}\right) e^{-in\theta}\,\mathrm{d}\theta \end{aligned} \tag{60}$$

Since the integrand has $2\pi$-periodicity, the integration range can be taken as an arbitrary interval of length $2\pi$. For any $L \in \mathbb{N}$, the function

$c : S^1 \to \mathbb{C}$ defines a Toeplitz matrix $\mathbf{T}_L$ [12] of order $L$ via the relation

$$(\mathbf{T}_L)_{ij} = c_{i-j}, \quad 1 \le i,j \le L \tag{61}$$

The function $c$ is called the *symbol* of the Toeplitz matrix $T_L$. The Fisher-Hartwig conjecture applies to Toeplitz matrices whose symbol verifies certain requirements (see Appendix B). For more technical details see Refs. [7, 12].

We shall be mainly interested in the case in which the Toeplitz matrix is $\mathbf{T}_L = \mu - (2\mathbf{A}_L - \mathbb{1})$, where $\mu$ is a spectral parameter and $\mathbf{A}_L$ is the correlation matrix of a block of $L$ spins. The determinant of $\mathbf{T}_L$ is the characteristic polynomial of $\mathbf{A}_L$, $D_L(\mu) \equiv \det(\mu + \mathbb{1} - 2\mathbf{A}_L) = \det \mathbf{T}_L$. For the XX model (or any model with a monotonic dispersion relation), it can be shown that

$$\begin{aligned} D_L(\mu) =& (2L\sin p_c)^{-2\beta^2}(\mu+1)^L \left(\frac{\mu+1}{\mu-1}\right)^{-Lp_c/\pi} \\ &\times G(1+\beta)^2 G(1-\beta)^2 \left[1 + \mathcal{O}(1)\right], \end{aligned} \tag{62}$$

with

$$\beta = \frac{1}{2\pi i}\log\left(\frac{\mu+1}{\mu-1}\right), \tag{63}$$

and

$$\begin{aligned} G(1+z)G(1-z) =& e^{-(1+\gamma)z^2} \\ &\times \prod_{n=1}^{\infty}\left[\left(1-\frac{z^2}{n^2}\right)^n e^{z^2/n}\right]. \end{aligned} \tag{64}$$

Eq. (62) is precisely the formula used by Jin and Korepin [7] for determining the asymptotic behaviour of the ground-state entanglement entropy of the XX model.

In order to complete the proof of the asymptotic formula for the entanglement entropy of the XX model (58), we shall now rewrite the general expression for the entanglement entropy (50) as a complex integral. Each eigenvalue $\nu_l$ in the right-hand side of Eq. (50) can be regarded as a residue for a suitable integral. Let us introduce $\tilde\nu \equiv 2\nu - 1 \in [-1,1]$ and

$$\begin{aligned} e(x,\tilde\nu) =& -\frac{x+\tilde\nu}{2}\log\left(\frac{x+\tilde\nu}{2}\right) \\ &- \frac{x-\tilde\nu}{2}\log\left(\frac{x-\tilde\nu}{2}\right), \end{aligned} \tag{65}$$

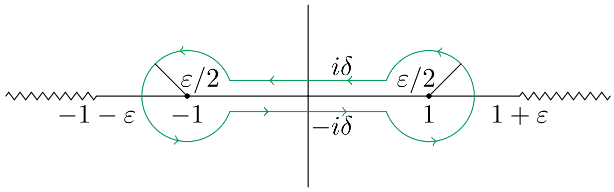


Figure 6. Integration path $\mathcal{C}(\varepsilon,\delta)$. Zigzag lines represent the branch cuts. The poles $\{\tilde\nu_1,\dots,\tilde\nu_L\}$ lie on the real line and on the interval $[-1,1]$.

so that $e(1,\tilde\nu)$ is equal to the Shannon binary entropy (51). The logarithm is analytic in the domain $\mathbb{C}\backslash\{z\in\mathbb{C} : \mathrm{Re}(z) \le 0 \text{ and } \mathrm{Im}(z) = 0\}$. Therefore the function $e(1+\varepsilon, z)$ has a logarithmic branch cut on the set $|\mathrm{Re}\, z| \ge 1+\varepsilon$ and no other singularities. Let $\mathcal{C}(\varepsilon,\delta)$ be a closed path that encircles all the zeros of $D_L(\mu)$, and such that $e(1+\varepsilon, z)$ is analytic over the path (*cf.* Fig. 6).

Let us briefly recall Cauchy's residue theorem [17]. Let $U$ be an open set, and $\mathcal{C}$ a closed curve in $U$ such that $\mathcal{C}$ is homologous to 0 in $U$. Let $f(z)$ be analytic on $U$ except for a finite number of points $z_1,\dots,z_L$. For our purposes we can assume that $\mathcal{C}$ has winding number equal to 1 around each of these singularities. Then the integral of $f(z)$ around $\mathcal{C}$ is given by

$$\oint_{\mathcal{C}} f(z)\,\mathrm{d}z = 2\pi i \sum_{k=1}^{L} \mathrm{Res}(f; z_k), \tag{66}$$

where $\mathrm{Res}(f;z_k)$ is the residue of $f(z)$ at $z_k$. If $f$ has a simple pole at $z_0$ and $g$ is holomorphic at $z_0$ (differentiable in a neighbour of $z_0$), then

$$\mathrm{Res}(fg; z_0) = g(z_0)\,\mathrm{Res}(f; z_0) \tag{67}$$

Finally, suppose $f(z_0) = 0$ but $f'(z_0) \ne 0$. Then $1/f$ has a pole of order 1 at $z_0$ and its residue is $1/f'(z_0)$. Therefore, if $f$ is of this kind and $g$ is holomorphic at $z_0$ we have

$$\begin{aligned} \mathrm{Res}\left(g\frac{\mathrm{d}\log f}{\mathrm{d}z}; z_0\right) &= \mathrm{Res}\left(g\frac{f'}{f}; z_0\right) \\ &= g(z_0)f'(z_0)\,\mathrm{Res}\left(\frac{1}{f}; z_0\right) \\ &= g(z_0)f'(z_0)\frac{1}{f'(z_0)} = g(z_0) \end{aligned} \tag{68}$$

We can now compute the line integral

$$\begin{aligned} I(\varepsilon,\delta) &= \oint_{\mathcal{C}(\varepsilon,\delta)} e(1+\varepsilon,\mu)\ \mathrm{d}\log D_L(\mu) \\ &= \oint_{\mathcal{C}(\varepsilon,\delta)} e(1+\varepsilon,\mu)\ \frac{D_L'(\mu)}{D_L(\mu)}\ \mathrm{d}\mu, \end{aligned} \tag{69}$$

whose only poles are simple, and correspond to the $L$ zeros of $D_L(\mu)$ at $\mu = \tilde{\nu}_k$ $(k = 1, \dots, L)$, and where $\mathcal{C}(\varepsilon,\delta)$ is the path sketched in Fig. 6. Its corresponding residues are

$$\mathrm{Res}\left( e(1+\varepsilon,\mu)\frac{\mathrm{d}\log D_L(\mu)}{\mathrm{d}\mu}; \tilde{\nu}_k \right) = e(1+\varepsilon,\tilde{\nu}_k), \tag{70}$$

then by the Cauchy's residue theorem we have

$$I(\varepsilon,\delta) = 2\pi i \sum_{k=1}^{L} e(1+\varepsilon,\tilde{\nu}_k). \tag{71}$$

If we now take the limits $\varepsilon,\delta \to 0^+$ we get the entanglement entropy:

$$\begin{aligned} \lim_{\varepsilon\to 0^+}\lim_{\delta\to 0^+} \frac{1}{2\pi i} I(\varepsilon,\delta) &= \sum_{k=1}^{L} e(1,\tilde{\nu}_k) \\ &= \sum_{l=1}^{L} H(\nu_l) = S_L \end{aligned} \tag{72}$$

Note that this cannot be done by integrating $e(1,\mu)$ directly, since the integration path would enclose branch cuts in $|\mu| \geq 1$. Instead, we have to move the branch cuts to $|\mu| \geq 1+\varepsilon$, take a path that does not cross those intervals (such as the one in Fig. 6) and then take the limit $\varepsilon \to 0$. The straight segments are taken outside the real line ($\delta > 0$) so that the poles do not lie on the integration path. The integral is independent of $\delta$, by the deformation theorem, as long as $\delta > 0$. However, once we replace $D_\mu$ by its asymptotic expression the integral does depend on $\delta$, and we have thus taken the $\delta \to 0^+$ limit.

We can now obtain the asymptotic form of the entanglement entropy [7]. For convenience, let us define

$$\Upsilon(\mu) := \sum_{n=1}^{\infty} \frac{n^{-1}\beta^2(\mu)}{n^2 - \beta^2(\mu)} \tag{73}$$

Taking the logarithmic derivative of $D_L(\mu)$ in Eq. (62), we get

$$\begin{aligned} \frac{\mathrm{d}\log D_L(\mu)}{\mathrm{d}\mu} =& -4\beta(\mu)\beta'(\mu)\log\left(2L\left|\sin p_c\right|\right) \\ &+ \left[\frac{1}{\mu+1} - \frac{p_c}{\pi}\left(\frac{1}{\mu+1} - \frac{1}{\mu-1}\right)\right] L \\ &+ 2\frac{\mathrm{d}}{\mathrm{d}\mu}\log\left[G(1+\beta)G(1-\beta)\right] \end{aligned} \tag{74}$$

Making use of the Eqs. (63) and (64) we have

$$\beta'(\mu) = \frac{1}{2\pi i}\left(\frac{1}{\mu+1} - \frac{1}{\mu-1}\right) = -\frac{1}{i\pi}\frac{1}{(1+\mu)(1-\mu)}, \tag{75}$$

and

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}z}\log\left[G(1+z)G(1-z)\right] \\ &= \frac{\mathrm{d}}{\mathrm{d}z}\left[-(1+\gamma)z^2 + \sum_{n=1}^{\infty} n\log\left(1-\frac{z^2}{n^2}\right) + \frac{z^2}{n}\right] \\ &= -2(1+\gamma)z + 2\sum_{n=1}^{\infty}\left(-n\frac{z/n^2}{1-z^2/n^2} + \frac{z}{n}\right) \\ &= -2(1+\gamma)z - 2\sum_{n=1}^{\infty} z\left(\frac{n}{n^2-z^2} - \frac{1}{n}\right) \\ &= -2z\left[(1+\gamma) + \sum_{n=1}^{\infty}\frac{z^2/n}{n^2-z^2}\right], \end{aligned} \tag{76}$$

so the logarithmic derivative of $D_L(\mu)$ results

$$\begin{aligned} \frac{\mathrm{d}\log D_L(\mu)}{\mathrm{d}\mu} \simeq& \left[\frac{1-p_c/\pi}{1+\mu} - \frac{p_c/\pi}{1-\mu}\right] L - \frac{4\beta(\mu)}{i\pi(1-\mu^2)} \\ &\times\left[\log L + \log(2\sin p_c) + (1+\gamma) + \Upsilon(\mu)\right]. \end{aligned} \tag{77}$$

We can now substitute the asymptotic form above into Eq. (69):

$$I(\varepsilon,\delta) = I_1(\varepsilon,\delta) + I_2(\varepsilon,\delta), \tag{78}$$

with

$$\begin{aligned} I_1(\varepsilon,\delta) =& L\oint_{\mathcal{C}(\varepsilon,\delta)} \mathrm{d}\mu\ e(1+\varepsilon,\mu)\left[\frac{1-p_c/\pi}{1+\mu} - \frac{p_c/\pi}{1-\mu}\right] \\ I_2(\varepsilon,\delta) =& -\frac{4}{i\pi}\oint_{\mathcal{C}(\varepsilon,\delta)} \mathrm{d}\mu\ e(1+\varepsilon,\mu)\frac{\beta(\mu)}{1-\mu^2} \\ &\times\left[\log L + \log(2\left|\sin p_c\right|) + (1+\gamma) + \Upsilon(\mu)\right] \end{aligned} \tag{79}$$

where the contour is taken as shown in Fig. 6. The first integral in the Eq. above can be evaluated by making use of the residue theorem and noting that the only residues are of the form (67). Indeed, let

$$I_1(\varepsilon,\delta) \equiv L \oint_{\mathcal{C}} e(1+\varepsilon,\mu)\left(\frac{1}{f_+(\mu)}+\frac{1}{f_-(\mu)}\right)\,\mathrm{d}\mu,$$
$$f_+(\mu)=\frac{1+\mu}{1-p_c/\pi},\quad f_-(\mu)=-\frac{1-\mu}{p_c/\pi}$$

Since $e(1+\varepsilon,\delta)$ is holomorphic in the region enclosed by $\mathcal{C}(\varepsilon,\delta)$ and the only singularities of the integrand are the simple poles of $f_\pm^{-1}(\mu)$ at $\mu=\mp 1$ we have

$$\begin{aligned}I_1(\varepsilon,\delta) =& 2\pi i L\left[e(1+\varepsilon,-1)\,\mathrm{Res}\left(\frac{1}{f_+},-1\right)\right.\\&\left.+e(1+\varepsilon,1)\,\mathrm{Res}\left(\frac{1}{f_-},1\right)\right]\end{aligned}$$

and taking the limit $\varepsilon\to 0$ the integral vanishes, since $e(1,\pm 1)=0$. In other words, the linear term in $L$ for the entanglement entropy vanishes when $L\to\infty$. The second integral can be written as follows:

$$I_2(\varepsilon,\delta)=\left(\int_{\circlearrowleft}+\int_{\rightarrow}+\int_{\circlearrowright}+\int_{\leftarrow}\right)(\cdots)\,\mathrm{d}\mu \tag{80}$$

where $\circlearrowleft$ and $\circlearrowright$ represent the right and left circular arcs respectively, while $\leftarrow$ and $\rightarrow$ represent the upper and lower straight segments. Note that the arcs are mapped to each other under $\mu\mapsto-\mu$. Since the integrand in $I_2$ is odd in $\mu$, the integrals along both arcs exactly cancel. Therefore, the entanglement entropy is given by

$$\begin{aligned}S_L=&\lim_{\varepsilon\to 0^+}\frac{2}{\pi^2}\left(\int_{1+i0}^{-1+i0}+\int_{-1+i0}^{1+i0}\right)e(1+\varepsilon,\mu)\\&\times\left[\log L+\log(2\left|\sin p_c\right|)+(1+\gamma)+\Upsilon(\mu)\right]\\&\times\frac{\beta(\mu)}{1-\mu^2}\,\mathrm{d}\mu,\end{aligned} \tag{81}$$

For further simplification, we shall make use of the fact that

$$\begin{aligned}\beta(x\pm i0)=&\frac{1}{2i\pi}\left[\log\left(\frac{1+x}{1-x}\right)\mp i(\pi\mp 0s)\right]\\=&-iW(x)\mp\frac{1}{2},\end{aligned} \tag{82}$$

for $x\in(-1,1)$ and

$$W(x)=\frac{1}{2\pi}\log\left(\frac{1+x}{1-x}\right) \tag{83}$$

The entanglement entropy can now be expressed as

$$\begin{aligned}S_L=&\frac{2}{\pi^2}\left[\log L+\log(2\sin p_c)+(1+\gamma)\right]\int_{-1}^{1}\frac{e(1,x)}{1-x^2}\,\mathrm{d}x\\&+\sum_{n=1}^{\infty}\frac{2n^{-1}}{\pi^2}\int\frac{e(1,x)}{1-x^2}\left[\frac{(1/2+iW(x))^3}{n^2-(1/2+iW(x))^2}\right.\\&\left.+\frac{(1/2-iW(x))^3}{n^2-(1/2-iW(x))^2}\right]\,\mathrm{d}x,\end{aligned} \tag{84}$$

where we have replaced $\Upsilon(\mu)$ by its definition (73). The first of these integrals can be computed exactly with elementary calculus methods, yielding

$$\begin{aligned}&\frac{2}{\pi^2}\int_{-1}^{1}\frac{e(1,x)}{1-x^2}\,\mathrm{d}x\\&=\frac{2}{\pi^2}\int_{-1}^{1}\frac{1}{1-x^2}\left[-\frac{1+x}{2}\log\left(\frac{1+x}{2}\right)\right.\\&\left.-\frac{1-x}{2}\log\left(\frac{1-x}{2}\right)\right]\,\mathrm{d}x=\frac{1}{3}\end{aligned} \tag{85}$$

The second integral in Eq. (84) can be expressed as

$$\begin{aligned}\Upsilon_0=&\sum_{n=1}^{\infty}\frac{n^{-1}}{\pi^2}\int_{-1}^{1}\mathrm{d}x\left[-\frac{1}{1-x}\log\frac{1+x}{2}\right.\\&\left.-\frac{1}{1+x}\log\frac{1-x}{2}\right]\\&\times\left[\frac{\left(\frac{1}{2}+iW(x)\right)^3}{n^2-\left(\frac{1}{2}+iW(x)\right)^2}+\frac{\left(\frac{1}{2}-iW(x)\right)^3}{n^2-\left(\frac{1}{2}-iW(x)\right)^2}\right]\end{aligned} \tag{86}$$

The asymptotic expression for the entanglement entropy is thus

$$S_L=\frac{1}{3}\log L+\frac{1}{3}\log\sin p_c+\frac{1}{3}\log 2+\frac{1+\gamma}{3}+\Upsilon_0 \tag{87}$$

Applying the trigonometric relation $\sin(\arccos x)=\sqrt{1-x^2}$ and the expression of $p_c$ for the XX model, $p_c=\arccos(\lambda/2)$, we get

$$S_L = \frac{1}{3}\log L + \frac{1}{6}\log\left[1-\left(\frac{\lambda}{2}\right)^2\right] + \frac{1}{3}\log 2 + \frac{1+\gamma}{3} + \Upsilon_0 \tag{88}$$

We can further simplify the expression for $\Upsilon_0$ (see Appendix C) and finally write

$$S_L = \frac{1}{3}\log L + \frac{1}{6}\log\left[1-\left(\frac{\lambda}{2}\right)^2\right] + \frac{1}{3}\log 2 + \Upsilon_1, \tag{89}$$

with

$$\Upsilon_1 = \int_0^\infty \left[-\frac{e^{-t}}{3t} - \frac{1}{t\sinh^2(t/2)} + \frac{\cosh(t/2)}{2\sinh^3(t/2)}\right]\mathrm{d}t \simeq 0.495018. \tag{90}$$

For the sake of clarification, let us summarize this last section. We have made use of the fact that the correlation matrix $\mathbf{A}$ of the XX model (or any suitable free fermion system) is a Toeplitz matrix, and thus the matrix $\mathbf{T} = \mu + \mathbb{1} - 2\mathbf{A}$ (whose determinant is the characteristic polynomial of $\mathbf{A}$) is also Toeplitz. Considering the case of the Fisher-Hartwig conjecture proven by Basor, we have expressed $\det \mathbf{T}$ for large values of $L$. Afterwards, we have rewritten the exact expression for the entanglement entropy as an integral along a complex contour involving $\det \mathbf{T}$. We have finally inserted the approximate expression of $\det \mathbf{T}$ furnished by the Fisher-Hartwig conjecture and evaluated the resulting integral. We have shown the dependence of the entanglement entropy with $L$ is logarithmic, with central charge $c = 1$, just like CFT predicted. Moreover, we have obtained the value of the constant term.

## VI. CONCLUSIONS AND OUTLOOK

In this paper we explore entanglement entropy as a quantitative measure for the amount of entanglement between a block of spins and the rest of a chain in the ground state. We regard the von Neumann entropy as the entanglement entropy and we focus on the XX chain for explicit computations. However, our results are easily extended [30] to any spin chain or one-dimensional free fermion system with a monotonic dispersion relation. Moreover, the procedures and results developed for the von Neumann entropy are applicable for the Rényi entropy as well with inessential modifications.

We have introduced the XX model, which consists on a chain of spin-$\frac{1}{2}$ particles with nearest neighbour interactions in an external magnetic field, whose only degrees of freedom correspond to the spin projections $|\uparrow\rangle$ and $|\downarrow\rangle$. The Jordan-Wigner transformation maps spin chains such as the XX model into free fermion systems. Fermionic creation and annihilation operators are defined by Eq. (8). These operators verify the canonical anticommutation relations, at the cost of making the interactions become non-local. The state with every spin down in the $z$-direction, $|\downarrow\cdots\downarrow\rangle$, is mapped into the fermionic vacuum state, $|0\cdots 0\rangle$. The resulting Hamiltonian is translationally invariant and preserves the number of fermions. It can thus be diagonalised via a Fourier transform. (In fact, even if the number of fermions were not preserved, the Hamiltonian could be diagonalised via an additional Bogoliubov transformation.) The energy of the $k$-th momentum mode is characteristic of each model and defines the dispersion relation, given by Eq. (17) for the XX model.

Through the correlation matrix method we have obtained an exact expression for the entanglement entropy of a block with $L$ spins in terms of the eigenvalues of the correlation matrix (50). This remarkable technique reduces the problem of diagonalising a $2^L \times 2^L$ density matrix $\rho_L$ to the polynomial problem of diagonalising the $L \times L$ correlation matrix $\mathbf{A}$.

In the case of the XX chain, the Fermi momentum $p_c$ is given by $p_c = \arccos(\lambda/2)$. If $\lambda > 2$ the magnetic field dominates over the hopping between spins, so that $\Lambda_k > 0$ for every $k$. The ground state is a product state (the vacuum state in the fermionic basis) and thus its entanglement entropy vanishes. On the other hand, if $0 \le \lambda < 2$, the hopping dominates, and the negative energy momentum modes become excited in the ground state. In the latter case, the ground state is a mixed state with non-zero entanglement entropy. At $\lambda = 2$ the ferromagnetic-critical phase transition takes place.

We have also studied the scaling of the entanglement entropy with the size of the system and its asymptotic behaviour. The scaling of the entanglement entropy as $L \to \infty$ is related with criticality and the system's invariance under conformal transformations. The entanglement entropy of one-dimensional fermionic systems behaves as $\mathcal{O}(\log L)$ in the gapless (critical) case, and as $\mathcal{O}(1)$ in the gapped (non-critical) one. Gapless systems have no natural scale and they are therefore invariant under dilations. If the Hamiltonian happens to be invariant under the full conformal group, the model is equivalent to a CFT in the low-energy regime. The universality class of a CFT is given by its central charge $c$, which can be computed by evaluating $S_L/\log L$ for $L \to \infty$. For the XX model this limit can in fact be calculated analytically, making use of the Fisher-Hartwig conjecture for the asymptotic behaviour of Toeplitz determinants. The central charge for this model happens to be $c = 1$, and hence the XX model falls into the universality class of a free boson [1].

A scaling variable $\mathcal{L}$, which depends on the value of the external magnetic field through $\lambda$, can be defined for the XX chain, so that the entanglement entropy of the block scales as

$$S_L \approx \begin{cases} \dfrac{\mathcal{L}}{\pi}\log\left(\dfrac{\pi}{\mathcal{L}}\right) & \text{if } \mathcal{L} \ll 1 \\ \dfrac{1}{3}\log\left(2\mathcal{L}\right) + \Upsilon_1 & \text{if } \mathcal{L} \gg 1 \end{cases}, \tag{91}$$

with

$$\mathcal{L} := L\sqrt{1-\left(\frac{\lambda}{2}\right)^2} \quad \text{for } \lambda < 2, \tag{92}$$

where $\Upsilon_1 \simeq 0.495018$ is a constant defined in terms of a definite integral that can be evaluated numerically. We could have obtained the Rényi entanglement entropy in a similar fashion. The results are in fact considerably resemblant to the von Neumann entanglement entropy, namely [7]

$$S_\alpha\left(\rho_L\right) = \begin{cases} \frac{1}{1-\alpha}\log\left[\left(\frac{\mathcal{L}}{\pi}\right)^\alpha + \left(1-\frac{\mathcal{L}}{\pi}\right)^\alpha\right], & \mathcal{L} \ll 1, \\ \frac{1+\alpha^{-1}}{6}\log\left(2\mathcal{L}\right) + \Upsilon_1^{\{\alpha\}}, & \mathcal{L} \gg 1. \end{cases} \tag{93}$$

For the sake of simplicity, we have only made explicit calculations for the XX chain. Nevertheless, the method exposed could be applied for any free fermion system, or a system equivalent to it via a Jordan-Wigner transformation, at zero temperature. The XY chain [1, 3, 8] is a more general model whose Hamiltonian can be written as

$$H_{\mathrm{XY}} = -\frac{1}{2}\sum_{l=0}^{N-1}\left(\frac{1+\gamma}{2}\sigma_l^x\sigma_{l+1}^x + \frac{1-\gamma}{2}\sigma_l^y\sigma_{l+1}^y + \lambda\sigma_l^z\right), \tag{94}$$

where the $\gamma$ parameter determines the degree of anisotropy of the spin-spin interaction in the XY plane. In particular, for $\gamma = 0$ we recover the XX model, whereas if $\gamma = 1$ it becomes the well-known quantum Ising model with a transverse magnetic field. The XY model with $\gamma \neq 0$ is critical for $\lambda = 1$. In this case, the entropy of a block scales as

$$S_{\mathrm{XY}}(L) \simeq \frac{1}{6}\log L + a\left(\gamma\right), \tag{95}$$

where $a(\gamma)$ is a function of $\gamma$ that depends on the Fermi momentum $p_c$. This behaviour corresponds to the scaling dictated by a CFT with $c = 1/2$, i.e. the universality class of a free fermion. In the non-critical case ($\lambda \neq 1$), the entanglement entropy saturates to a constant. Moreover, the exact relation between the entropies of the XY model and the quantum Ising model was found in Ref. [19]. Making use of this relation it is possible, among other results, to obtain the effective central charge of the random XY chain, as well as the additive constant of the entropy for the critical homogeneous quantum Ising chain. Other models for which similar techniques can be applied include the XXZ model [1] and su(1|1) supersymmetric chains [11, 12].

There are several open lines of research suggested by the present work, namely:

- The scaling of the entanglement entropy for thermal –non-zero temperature– states of the XX model has been recently estimated through CFT techniques and numerical simulations in Ref. [20].

- The search for exact expressions for the entanglement entropy for models beyond quasifree and conformally invariant systems [3], both in one and higher dimensions, is also an open area of research.

- The asymptotic behaviour of the entanglement entropy for models whose correlation matrix is not Toeplitz, or does not verify the conditions required by proven cases of the Fisher-Hartwig conjecture, is tough to determine. However, for some of these models their connection with a suitable CFT can be exploited to derive the asymptotic behaviour of the entanglement entropy. This idea has been successfully applied to the inhomogeneous XX chain so-called rainbow chain in Ref. [21]. In fact, the connection between general inhomogeneous XX chains and quasi-exactly solvable models has been recently studied in Ref. [13].

- The notion of area law (i.e. the saturation of $S_L$ for $L \to \infty$) acquires considerably more complexity for higher dimensions, where the boundary of a region becomes a non-trivial object. In the present state-of-the-art [3], the question whether the entanglement entropy of a (higher-dimensional) subregion fulfills an area law has only been solved rigorously for quasifree bosonic and fermionic models at zero temperature. Even in such models, the technical details involved are quite intricate. These models can be considered as a "laboratory" for more general systems. Area laws are not always satisfied, and they are expected to hold whenever one has a gapped and local model, when a length scale is provided by the correlation length, as "laboratory" models and numerical studies suggest. The sufficient conditions to ensure that a higher-dimensional critical system satisfies an area law are still undetermined. Area laws seem to be connected with geometry, as it was recently emphasized in Ref. [22].

- Finally, the above results may provide new perspectives for problems related with quantum entanglement in quantum information theory, many-body systems or high-energy physics.

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## Appendix A: Conformal field theory

In general, critical models exhibit a divergent correlation length, thus they become scale invariant and allow for a general description of conformal field theories [3]. According to the universality hypothesis, the microscopic details become irrelevant for numerous crucial properties, which depend only on basic properties such as the symmetry of the system or the spatial dimension. Models belonging to the same universality class are characterized by the same fixed-point Hamiltonian –a Hamiltonian that is mapped to itself– under renormalization transformations, which is invariant under general rotations. Conformal field theory provides a description for such continuum models, which have the symmetries of the conformal group (including translations, rotations and scalings). As we already mentioned, the universality class is characterized by the central charge $c$, a parameter that roughly quantifies the "degrees of freedom" of the theory. More specifically, $c$ is an operator that commutes with all the other symmetry operators, and the adjective "central" is referred to the centre of the symmetry group. For free bosons and the XX model $c = 1$, whereas the Ising universality class has $c = 1/2$.

Knowing that a model can be described by a conformal field theory (CFT) grants robust methods to compute universal properties, as well as entanglement entropies of subsystems. This methods are available for (1+1)-dimensional systems, i.e. with one spatial dimension. To start with, we note that the powers of the reduced density matrix $\rho_L^n$ can be computed for any positive integer $n$. The series

$$\mathrm{tr}\left[\rho_L^n\right] = \sum_j \lambda_j^n \tag{A1}$$

where $\{\lambda_j\}_{j=1}^{L}$ are the eigenvalues of of $\rho_L$, is absolute convergent and analytic. As the derivative exists, we can make use of the "replica trick" to compute the entanglement entropy, namely,

$$S(\rho_L) = \lim_{n\to 1} -\frac{\partial}{\partial n}\,\mathrm{tr}\left[\rho_L^n\right] \tag{A2}$$

Indeed,

$$\begin{aligned}\frac{\partial}{\partial n}\,\mathrm{tr}\left[\rho_L^n\right] &= \frac{\partial}{\partial n}\sum_{i=1}^{L}\lambda_i^n = \frac{\partial}{\partial n}\sum_{i=1}^{L} e^{n\log\lambda_i}\\ &= \sum_{i=1}^{L}\log\lambda_i\; e^{n\log\lambda_i} \xrightarrow{n\to 1} \sum_{i=1}^{L}\lambda_i\log\lambda_i\end{aligned}$$

In $1+1$ dimensions this leads to the expression

$$S\left(\rho_L\right) = \frac{c}{3}\log\left(\frac{L}{a}\right) + \mathcal{O}(1) \tag{A3}$$

where $L$ is the length of the block, $a$ is an ultraviolet cut-off, corresponding to a lattice spacing, to avoid ultraviolet divergence. Moreover, if one is close to the critical point, where the correlation length $\xi > 0$ is large but finite, one can typically still describe the system by a CFT. The dominant term of the entanglement entropy is then

$$S(\rho_L) \sim \frac{c}{3}\log\left(\frac{\xi}{a}\right) \tag{A4}$$

The modern theory of continuous phase transitions is based on quantum field theory (QFT). This apparently unrelated subjects are connected by the renormalization group (RG) theory [10]. Let us consider a system whose Hamiltonian $H(\lambda)$ depends on a tunable experimental parameter $\lambda$ (the magnetic field strength in the case of the XX model or the Ising model). At the critical point $\lambda = \lambda_c$, the Hamiltonian undergoes a continuous phase transition. Close to $\lambda_c$, the correlation length (the only relevant scale for long-distance physics) behaves like $\xi = |\lambda - \lambda_c|^{-\nu}$, diverging at $\lambda_c$. Hence, at the critical point the system is scale invariant. The RG transformations are, roughly speaking, practical implementations of scale transformations. As we mentioned, the universality hypothesis (in terms of RG) means that different Hamiltonians sharing the same universal characteristics flow to the same fixed point, which completely determines the long-distance behaviour. For instance, consider a lattice model whose Hamiltonian is invariant under translations multiple of the lattice spacing; whereas the resulting fixed point Hamiltonian is typically invariant under arbitrary translations, and hence it can be described with a continuum field theory. For the same reason, the critical point Hamiltonian is usually rotationally invariant as well.

These transformations of translations, rotations and scaling form a group. We can exploit its group properties to infer the form of certain magnitudes. As an example, consider the correlator of two scalar observables $\langle\phi(\mathbf{r}_1) - \phi(\mathbf{r}_2)\rangle$.

- By translational invariance, it can be only a function of $\mathbf{r}_1 - \mathbf{r}_2$.
- By rotational invariance, it can depend only upon the modulus $\|\mathbf{r}_1 - \mathbf{r}_2\|$.
- For a scale transformation $\mathbf{r} \mapsto b\mathbf{r}$, it must behave as

$$\langle\phi(\mathbf{r}_1)\phi(\mathbf{r}_2)\rangle = b^{2\Delta_\phi}\,\langle\phi(b\mathbf{r}_1)\phi(b\mathbf{r}_2)\rangle\,, \tag{A5}$$

so that the the identity scaling $b = 1$ leaves the correlator unchanged, and the action of a scale transformation $b$ and its inverse $1/b$ returns to the original correlator. The exponent $\Delta_\phi$ is called scaling dimension of the field $\phi$. These three conditions can be true if and only if

$$\langle\phi(\mathbf{r}_1)\phi(\mathbf{r}_2)\rangle = \|\mathbf{r}_1 - \mathbf{r}_2\|^{-2\Delta_\phi} \tag{A6}$$

apart from a normalization constant we set equal to 1.

Fixed point Hamiltonians invariant under translations, rotations and scaling transformations usually turn out to have the symmetry of the larger conformal group –the set of transformations that do not change the angles between two arbitrary curves crossing each other in some point. In a two-dimensional Euclidean space (or a 1 + 1-dimensional spacetime) this invariance has outstanding consequences. In fact, it can be proved that all the analytic functions $f(z)$, with $z = x + iy$, are conformal transformations [10]. The resulting symmetry group is infinite-dimensional and everything can be calculated, in principle, analytically. For instance, under a transformation of the form $z \mapsto w = w(z)$, equation (A5) can be generalized to a space-dependent scale factor $b(z) = \mathrm{d}w/\mathrm{d}z \equiv w'(z)$, obtaining

$$\langle \phi(z_1)\,\phi(z_2)\rangle = \left(\left|w'(z_1)\,w'(z_2)\right|\right)^{2\Delta_\phi} \times \langle \phi(w(z_1))\,\phi(w(z_2))\rangle \tag{A7}$$

This equation relates the correlation function of a scalar field on the plane, given by equation (A6), to the one in an arbitrary geometry, e.g. in a torus.

We need to introduce the so-called stress tensor $T^{\mu\nu}$. Under an arbitrary transformation $x^\mu \to x^\mu + \epsilon^\mu$, the Euclidean action (the Hamiltonian for classical systems) changes as

$$S \to S + \delta S, \quad \delta S =: \int \mathrm{d}^2x\, T^{\mu\nu}\partial_\mu\epsilon_\nu \tag{A8}$$

The universality class (of minimal unitary models) of two-dimensional CFT is characterized by the central charge, which assumes only discrete values. From the knowledge of the central charge $c$ we can compute all the critical properties of the model, such as the critical exponents [10].

Consider a subsystem $A$ formed by the points $x$ in the disjoint intervals $(u_1, v_1), \ldots, (u_N, v_N)$. An expression of the reduced density matrix $\rho_A$ may be found by stitching together those points which are not in $A$. Then $\mathrm{tr}\,\rho_A^n$ can be computed by making $n$ copies of the above and sewing them cyclically along the cuts. Then

$$\mathrm{tr}\,\rho_A^n = \frac{Z_n(A)}{Z^n} \tag{A9}$$

where $Z$ is the partition function (that ensures $\mathrm{tr}\,\rho = 1$) and $Z_n(A)$ is the path integral on the n-sheeted surface.

We now consider that $A$ is a single interval of length $L$ in an infinitely long one-dimensional quantum system, at zero temperature (e.g. the asymptotic behaviour of the XX model). The ratio (A9) is given by $\langle 0\rangle_{\mathcal{R}_n}$, the vacuum expectation value in the $n$-sheeted surface. CFT allows to obtain this expectation value from just knowing how it transforms under a general conformal transformation [10]. This is formally given by $\langle T(w)\rangle_{\mathcal{R}_n}$, where $T(w)$ is the holomorphic stress tensor. To obtain $\langle T(w)\rangle_{\mathcal{R}_n}$, we need to map the $n$-sheeted surface onto a geometry where the mean value of the stress tensor is known, and then make use of the transformation law,

$$T(w) = \left(z''\right)^2 T(z) + \frac{c}{12}\,\frac{z'''z' - \frac{3}{2}z''^2}{z'^2} \tag{A10}$$

We need to map the $n$-sheeted surface $\mathcal{R}_n$ to the $z$-plane $\mathbf{C}$, where by translational and rotational invariance $\langle T(z)\rangle_{\mathbf{C}} = 0$. This mapping is $w \mapsto z(w) = [(w-u)/(w-v)]^{1/n}$, and hence, calculating the derivatives we obtain

$$\langle T(w)\rangle_{\mathcal{R}_n} = \frac{c\left(1-(1/n)^2\right)}{24}\,\frac{(v-u)^2}{(w-u)^2(w-v)^2} \tag{A11}$$

The correlator of $T$ with two primary operators $\Phi_n(u)$ and $\Phi_{-n}(v)$, with the same complex scaling dimensions $\Delta_n = \overline{\Delta}_n = (c/24)[1-(1/n)^2]$, is given by the conformal Ward identity [10]:

$$\langle T(w)\Phi_n(u)\Phi_{-n}(v)\rangle_{\mathbf{C}} = \frac{\Delta_n}{(w-u)^2(w-v)^2(v-u)^{2\Delta_n-2}(\bar{v}-\bar{u})^{2\Delta_n}} \tag{A12}$$

where $\Phi_{\pm n}$ are normalized so that $\langle\Phi_n(u)\Phi_{-n}(v)\rangle_{\mathbf{C}} = |v-u|^{-4\Delta_n}$. In the above we are assuming that $w$ is a complex coordinate in a single sheet $\mathbf{C}$, which is now decoupled from the others. Therefore

$$\langle T(w)\rangle_{\mathcal{R}_n} = \frac{\langle T(w)\Phi_n(u)\Phi_{-n}(v)\rangle_{\mathbf{C}}}{\langle\Phi_n(u)\Phi_{-n}(v)\rangle_{\mathbf{C}}} \tag{A13}$$

The insertion of $T(w)$ on each sheet is given by (A12). To insert it on all the sheets, the right-hand side gets multiplied by a factor $n$. As all the properties under conformal transfromations are determined by (A12), we conclude that (apart from a overall constant) $\mathrm{tr}\,\rho_L^n$ behaves as the correlation function of a primary operator $\Phi_n$ with $\Delta_n = \overline{\Delta}_n = (c/24)[1-(1/n)^2]$, namely,

$$\mathrm{tr}\,\rho_L^n = c_n \left(\frac{v-u}{a}\right)^{-(c/6)(n-1/n)} \quad \text{(A14)}$$

where the exponent is $-4n\Delta_n$ and $a$ is inserted to make the final result dimensionless. Since $\mathrm{tr}\,\rho_L = 1$, $c_1$ must be unity. We can now make use of the replica trick (A2) and finally show that

$$S_L = \frac{c}{3}\log\left(\frac{L}{a}\right) + c_1' \quad \text{(A15)}$$

where the constant $c_1'$ is not universal.

## Appendix B: Fisher-Hartwig conjecture

The Fisher-Hartwig conjecture applies to Toeplitz matrices whose symbol verifies certain requirements that we shall describe in the following paragraphs. More precisely, $c$ should be of the form

$$c(z) = b(z)\prod_{r=1}^{R} t_{\beta_r}\left(e^{i(\theta-\theta_r)}\right)\left[2-2\cos\left(\theta-\theta_r\right)\right]^{\alpha_r}, \quad \text{(B1)}$$

where $\mathrm{Re}\alpha_r > -1/2$, $b : S^1 \to \mathbb{C}$ is a non-vanishing smooth function with zero winding number, and

$$t_\beta(z) = e^{i\beta(\theta-\pi)}, \quad \theta \equiv \arg_{[0,2\pi)} z. \quad \text{(B2)}$$

Note that, unless $\beta$ is an integer, $t_\beta\left(e^{i(\theta-\theta_0)}\right)$ has a single jump discontinuity at $z = e^{i\theta} = e^{i\theta_0}$. Indeed, $t_\beta(z) = e^{-i\beta\pi}e^{i\beta\arg z}$ has a jump discontinuity on the positions real axis, since $\arg z$ jumps from $2\pi$ to 0 as we cross the positions real axis from $\mathrm{Im}\,z < 0$ to $\mathrm{Im}\,z > 0$. Consequently, $t_\beta\left(e^{i(\theta-\theta_0)}\right)$ (which is a function of $\theta$) has a jump discontinuity for $\theta = \theta_0 + 2k\pi$ ($k \in \mathbb{Z}$), i.e., $e^{i\theta} = e^{i\theta_0}$.

If the symbol $c$ satisfies Eq. (B1), we denote by $\ell_n$ ($n \in \mathbb{Z}$) the $n$th Fourier coefficient of $\log b$ (which is well defined and smooth, from the smoothness of $b$ and the assumption on its winding number), and introduce

$$b_\pm(z) := \exp\left(\sum_{n=1}^{\infty}\ell_{\pm n} z^{\pm n}\right), \quad z \in S_1. \quad \text{(B3)}$$

It can be shown that $b_+$ (resp. $b_-$) can be analytically prolonged to the interior (resp. exterior) of the unit circle. It also follows from the definition of $b_\pm$ that on the unit circle we have the Wiener-Hopf decomposition.

$$b(z) = e^{\ell_0} b_+(z) b_-(z), \quad z \in S^1 \quad \text{(B4)}$$

Let us also set

$$E[b] := \exp\left(\sum_{n=1}^{\infty} n\, \ell_n \ell_{-n}\right), \quad \text{(B5)}$$

and

$$\begin{aligned} E :=& E[b]\prod_{r=1}^{R} b_+\left(e^{i\theta_r}\right)^{\beta_r-\alpha_r} b_-\left(e^{i\theta_r}\right)^{-\beta_r-\alpha_r} \\ &\times \prod_{1\le s\ne r\le R}\left(1-e^{i(\theta_s-\theta_r)}\right)^{(\alpha_r+\beta_r)(\beta_s-\alpha_s)} \\ &\times \prod_{r=1}^{R}\frac{G\left(1+\alpha_r+\beta_r\right)G\left(1+\alpha_r-\beta_r\right)}{G\left(1+2\alpha_r\right)}, \end{aligned} \quad \text{(B6)}$$

where the Barnes $G$-function (or double Gamma function) [18] is the entire function defined by

$$\begin{aligned} G(1+z) =& (2\pi)^{z/2} e^{-(z+1)(z/2)-\gamma\left(z^2/2\right)} \\ &\times \prod_{n=1}^{\infty}\left[\left(1+\frac{z}{n}\right)^n e^{-z+z^2/2n}\right], \end{aligned} \quad \text{(B7)}$$

and $\gamma = 0.5770836\ldots$ is the Euler-Mascheroni constant. The Fisher-Hartwig conjecture states that if $\mathbf{T}_L$ is the Toeplitz matrix with symbol (B1) then when $L \to \infty$ we have

$$\det \mathbf{T}_L = e^{i\ell_0} L^M E\left[1+\mathcal{O}\left(1\right)\right], \quad \text{(B8)}$$

with

$$M = \sum_{r=1}^{R}\left(\alpha_r^2 - \beta_r^2\right). \quad \text{(B9)}$$

The above conjecture has actually been proven in Refs. [15] and [16] in the case

$$\alpha_r = 0, \quad |\mathrm{Re}\beta_r| < \frac{1}{2}, \quad r = 1,\ldots,R, \quad \text{(B10)}$$

which, as we shall next see, is the relevant one for our purposes. Moreover, we shall only need to consider the case in which $b$ is a constant (i.e.

independent of $\theta$). The Fisher-Hartwig conjecture then simplifies considerably, as

$$\ell_n = \ell_0\ \delta_{0n} \Rightarrow b_\pm = E[b] = 1, \quad e^{\ell_0} = b, \tag{B11}$$

and thus

$$\det \mathbf{T}_L = b^L L^M E\left[1 + \mathcal{O}\left(1\right)\right], \tag{B12}$$

with

$$M = -\sum_{r=1}^{R} \beta_r^2, \tag{B13}$$

and

$$E = \prod_{1\le s<r\le R} \left[2\left|\sin\left(\frac{\theta_r-\theta_s}{2}\right)\right|\right]^{2\beta_r\beta_s} \times \prod_{r=1}^{R} G(1+\beta_r)G(1-\beta_r). \tag{B14}$$

Note as well that the product of the Barnes functions reduces to

$$G(1+z)G(1-z) = e^{-(1+\gamma)z^2} \times \prod_{n=1}^{\infty}\left[\left(1-\frac{z^2}{n^2}\right)^n e^{z^2/n}\right] \tag{B15}$$

We shall be mainly interested in the case in which $\mathbf{T}_L = \mu - (2\mathbf{A}_L - \mathbb{1})$, where $\mu$ is a spectral parameter and $\mathbf{A}_L$ is the correlation matrix of a block of $L$ spins. The determinant of $\mathbf{T}_L$ is the characteristic polynomial of $\mathbf{A}_L$, $D_L(\mu) \equiv \det(\mu + \mathbb{1} - 2\mathbf{A}_L) = \det \mathbf{T}_L$. When the chain's dispersion relation is monotonic [12] in the interval $[0,\pi]$ (like the one represented in Fig. 3) we have

$$(\mathbf{A}_L)_{jk} = \frac{\sin\left[x_c(j-k)\right]}{\pi(j-k)} = \frac{1}{2\pi}\int_{-x_c}^{x_c} e^{-i(j-k)\theta}\ \mathrm{d}\theta \tag{B16}$$

Indeed,

$$\begin{aligned}\int_{-x_c}^{x_c} e^{-i(j-k)\theta}\ \mathrm{d}\theta &= \int_{-x_c}^{x_c} \cos\left[(j-k)\theta\right]\ \mathrm{d}\theta \\ &\quad - i\underbrace{\int_{-x_c}^{x_c} \sin\left[(j-k)\theta\right]\ \mathrm{d}\theta}_{\to 0} \\ &= \left.\frac{\sin\left[(j-k)\theta\right]}{j-k}\right|_{-x_c}^{x_c} \\ &= 2\frac{\sin\left[x_c(j-k)\right]}{j-k} = 2\pi\left(\mathbf{A}_L\right)_{jk}\end{aligned}$$

where $x_c \in [0,\pi]$ is the Fermi momentum [11]

$$x_c = \frac{2\pi k_c}{N} \in (0,\pi), \tag{B17}$$

with $\varepsilon(x_c) = \lambda$ for the dispersion relation $\varepsilon(x)$ and chemical potential $\lambda$. For the XX model $\varepsilon(x) = 2\cos(x)$ and $x_c = \arccos(\lambda/2)$. The symbol of the Toeplitz matrix $\mathbf{A}_L$ is hence

$$f\left(e^{i\theta}\right) = \begin{cases} 1, & \text{if } -x_c<\theta<x_c, \\ 0, & \text{if } x_c<\theta<2\pi-x_c, \end{cases} \tag{B18}$$

and that of $\mathbf{T}_L$ is thus given by

$$c\left(e^{i\theta}\right) = \begin{cases} \mu-1, & \text{if } -x_c<\theta<x_c, \\ \mu+1, & \text{if } x_c<\theta<2\pi-x_c. \end{cases} \tag{B19}$$

Note that $c$ has two jump discontinuities on the unit circle at the points $e^{\pm i x_c}$. We shall now show that

$$c\left(e^{i\theta}\right) = b\left(e^{i\theta}\right) t_\beta\left(e^{i(\theta+x_c)}\right) t_{-\beta}\left(e^{i(\theta-x_c)}\right) \tag{B20}$$

for suitable $\beta$ and $b(z)$. Indeed, we have

$$-x_c < \theta < 2\pi - x_c \Leftrightarrow 0 < \theta + x_c < 2\pi$$

so that

$$t_\beta\left(e^{i(\theta+x_c)}\right) = e^{i\beta(\theta+x_c-\pi)}$$

On the other hand, if $-x_c < \theta < x_c$ then

$$0 \le 2(\pi - x_c) < \theta - x_c + 2\pi < 2\pi,$$

and therefore

$$t_{-\beta}\left(e^{i(\theta-x_c)}\right) = e^{-i\beta(\theta-x_c+\pi)};$$

while for $x_c < \theta < 2\pi - x_c$ we have

$$0 < \theta - x_c < 2(\pi - x_c) \le 2\pi,$$

which implies

$$t_{-\beta}\left(e^{i(\theta-x_c)}\right) = e^{-i\beta(\theta-x_c-\pi)}.$$

Hence

$$t_\beta\left(e^{i(\theta+x_c)}\right)t_{-\beta}\left(e^{i(\theta-x_c)}\right) = \begin{cases} e^{2i\beta(x_c-\pi)}, & -x_c<\theta<x_c, \\ e^{2i\beta x_c}, & x_c<\theta<2\pi-x_c. \end{cases} \tag{B21}$$

In order for Eqs. (B19) and (B20) to hold we must therefore verify

$$be^{2i\beta(x_c-\pi)} = \mu - 1, \quad be^{2i\beta x_c} = \mu + 1, \tag{B22}$$

or equivalently

$$e^{2i\beta\pi} = \frac{\mu+1}{\mu-1}, \quad b = (\mu+1)e^{-2i\beta x_c}. \tag{B23}$$

These equations admit an infinite number of solutions $(\beta, b)$ provided that $\mu \neq \pm 1$. However, for our purposes we can conveniently choose the solutions

$$\beta = \frac{1}{2\pi i}\log\left(\frac{\mu+1}{\mu-1}\right), \quad b = (\mu+1)\left(\frac{\mu+1}{\mu-1}\right)^{-x_c/\pi} \tag{B24}$$

where the complex logarithm is $\log z := \log|z| + i\arg_{(-\pi,\pi]} z$, and $z^a := e^{a\log z}$. Let us remark that $b$ is a non-vanishing constant. It is also important to observe that if $\mu \in [-1,1]$ then

$$|\mathrm{Re}\beta| = \frac{1}{2\pi}\arg_{(-\pi,\pi]}\left(\frac{\mu+1}{\mu-1}\right) < \frac{1}{2}, \tag{B25}$$

since by definition $-\pi < \arg_{(-\pi,\pi]} z \leq \pi$ and

$$\arg_{(-\pi,\pi]}\left(\frac{\mu+1}{\mu-1}\right) = \pi \Leftrightarrow \frac{\mu+1}{\mu-1} \in (-\infty, 0) \Leftrightarrow \mu \in (-1,1). \tag{B26}$$

The Fisher-Hartwig conjecture can thus be applied provided that $\mu$ lies outside the interval $[-1,1]$, with $R = 1$, $\alpha_1 = 0$, $M = -2\beta^2$ and

$$E = (2\sin x_c)^{-2\beta^2} G(1+\beta)^2 G(1-\beta)^2. \tag{B27}$$

By Eqs. (B12) and (B24), when $L \to \infty$ the characteristic polynomial is given by

$$\begin{aligned} D_L(\mu) =& (2L\sin x_c)^{-2\beta^2}(\mu+1)^L\left(\frac{\mu+1}{\mu-1}\right)^{-Lx_c/\pi} \\ &\times G(1+\beta)^2 G(1-\beta)^2\left[1 + \mathcal{O}(1)\right] \end{aligned} \tag{B28}$$

## Appendix C: Simplification of the expression for $\Upsilon_0$

In this Appendix we shall simplify the formula of $\Upsilon_0$. Let us introduce the function [18]

$$\begin{aligned} \psi(z) &:= \frac{\mathrm{d}}{\mathrm{d}z}\log\Gamma(z) \\ &= -\gamma + \sum_{n=0}^{\infty}\left(\frac{1}{n+1} - \frac{1}{n+z}\right), \end{aligned} \tag{C1}$$

where $\Gamma(z)$ is the well-known Gamma function. This function satisfies the recurrence relation

$$\psi(z+1) = \psi(z) + \frac{1}{z} \tag{C2}$$

Therefore, we have

$$\begin{aligned} &\sum_{n=1}^{\infty}\left(\frac{1}{n+z} - \frac{1}{n}\right) = \sum_{n=1}^{\infty}\frac{1}{n+z} - \sum_{n=0}^{\infty}\frac{1}{n+1} \\ &= \sum_{n=0}^{\infty}\left(\frac{1}{n+z} - \frac{1}{n+1}\right) - \frac{1}{z} = -\gamma - \psi(z) - \frac{1}{z} \\ &= -\gamma - \psi(z+1) \end{aligned} \tag{C3}$$

Let

$$f(z) := \sum_{n=1}^{\infty}\frac{z^3}{n(n^2-z^2)}, \tag{C4}$$

with $z := 1/2 + iW(x)$. Note that $\bar{z} = 1 - z$, and thus

$$\begin{aligned} \mathrm{Re}\, f(z) &= \frac{1}{2}\left(f(z) + \overline{f(z)}\right) \\ &= \frac{1}{2}\left(f(z) + f(\bar{z})\right) \\ &= \frac{1}{2}\left(f(z) + f(1-z)\right) \end{aligned} \tag{C5}$$

To compute $f(z)$, we make use of the identity

$$\frac{z^3}{n(n^2-z^2)} = \frac{z}{2}\left(\frac{1}{n+z} - \frac{1}{n}\right) + \frac{z}{2}\left(\frac{1}{n-z} - \frac{1}{n}\right) \tag{C6}$$

which combined with (C3) implies

$$\begin{aligned} f(z) =& \frac{z}{2}\left(-\gamma - \psi(1+z)\right) \\ &+ \frac{z}{2}\left(-\gamma - \psi(1-z)\right) \\ =& -\gamma z - \frac{z}{2}\left(\psi(1+z) + \psi(1-z)\right) \\ =& -\gamma z - \frac{z}{2}\left(\psi(z) + \psi(1-z)\right) - \frac{1}{2}, \end{aligned} \tag{C7}$$

where at the last step we have made use of the recurrence relation (C2), and hence

$$f(z)+f(1-z)=-\gamma-\frac{1}{2}\left(\psi(z)+\psi(1-z)\right)-1. \quad \text{(C8)}$$

Substituting this result into Eq. (86) we obtain

$$\begin{aligned}\Upsilon_0=&\frac{1}{\pi^2}\int_{-1}^{1}\left[-\frac{1}{1-x}\log\frac{1+x}{2}-\frac{1}{1+x}\log\frac{1-x}{2}\right]\\ &\times\left[-\gamma-1-\frac{1}{2}\psi\left(\frac{1}{2}-iW(x)\right)\right.\\ &\left.-\frac{1}{2}\psi\left(\frac{1}{2}+iW(x)\right)\right]\mathrm{d}x\\ =&\Upsilon_1-\frac{1+\gamma}{3},\end{aligned} \quad \text{(C9)}$$

with $\Upsilon_1$ given by

$$\begin{aligned}\Upsilon_1=&-\frac{1}{2\pi^2}\int_{-1}^{1}\mathrm{d}x\left[-\frac{1}{1-x}\log\frac{1+x}{2}\right.\\ &\left.-\frac{1}{1+x}\log\frac{1-x}{2}\right]\\ &\times\left[\psi\left(\frac{1}{2}-iW(x)\right)+\psi\left(\frac{1}{2}+iW(x)\right)\right].\end{aligned} \quad \text{(C10)}$$

We now perform a change of variable using

$$w=\frac{1}{2\pi}\log\left(\frac{1+x}{1-x}\right)\Leftrightarrow x=\tanh(\pi w), \quad \text{(C11)}$$

which yields

$$\begin{aligned}\Upsilon_1=&-\frac{1}{\pi}\int_{-\infty}^{\infty}\left[\log\left(2\cosh(\pi w)\right)-\pi w\tanh(\pi w)\right]\\ &\times\left[\psi\left(\frac{1}{2}-iw\right)+\psi\left(\frac{1}{2}+iw\right)\right]\ \mathrm{d}w\\ =&-\frac{2}{\pi}\int_0^{\infty}\mathrm{d}w\left[\log(2\cosh(\pi w))-\pi w\tanh(\pi w)\right]\\ &\times\left[\psi\left(\frac{1}{2}-iw\right)+\psi\left(\frac{1}{2}+iw\right)\right]\ \mathrm{d}w,\end{aligned} \quad \text{(C12)}$$

where we have taken into account that $\cosh x$ is even, that $\tanh x$ is odd and that $\psi(1+z)+\psi(1-z)$ is even by construction. We now note that

$$\begin{aligned}&\log\left[2\cosh(\pi w)\right]-\pi w\tanh(\pi w)\\ &=\left(1-\frac{\mathrm{d}}{\mathrm{d}\alpha}\right)\log\left(1+e^{-2\pi w\alpha}\right)\Big|_{\alpha=1},\end{aligned} \quad \text{(C13)}$$

and that, by definition,

$$\begin{aligned}&\psi\left(\frac{1}{2}-iw\right)+\psi\left(\frac{1}{2}+iw\right)\\ &=i\frac{\mathrm{d}}{\mathrm{d}w}\log\left(\frac{\Gamma(1/2-iw)}{\Gamma(1/2+iw)}\right).\end{aligned} \quad \text{(C14)}$$

Making use of the following expression for the logarithm of the Gamma function [18]

$$\log\Gamma(z)=\int_0^{\infty}\left[z-1-\frac{1-e^{-(z-1)t}}{1-e^{-t}}\right]\frac{e^{-t}}{t}\ \mathrm{d}t, \quad \text{(C15)}$$

we can write

$$\begin{aligned}&\log\left(\frac{\Gamma(1/2-iw)}{\Gamma(1/2+iw)}\right)\\ &=-i\int_0^{\infty}\left[2we^{-t}-\frac{\sin(wt)}{\sinh(t/2)}\right]\frac{1}{t}\ \mathrm{d}t,\end{aligned} \quad \text{(C16)}$$

Therefore $\Upsilon_1$ is given by the double integral

$$\begin{aligned}\Upsilon_1=&-\frac{2}{\pi}\int_0^{\infty}\mathrm{d}w\int_0^{\infty}\mathrm{d}t\\ &\times\left\{\log\left[2\cosh(\pi w)\right]-\pi w\tanh(\pi w)\right\}\\ &\times\left(2\frac{e^{-t}}{t}-\frac{\cos(wt)}{\sinh(t/2)}\right)\end{aligned} \quad \text{(C17)}$$

The integrals in $w$ can be performed analytically with `Mathematica`, namely

$$\int_0^{\infty}\left\{\log\left[2\cosh(\pi w)\right]-\pi w\tanh(\pi w)\right\}\mathrm{d}w=\frac{\pi}{12} \quad \text{(C18)}$$

and

$$\begin{aligned}&\int_0^{\infty}\left\{\log\left[2\cosh(\pi w)\right]-\pi w\tanh(\pi w)\right\}\cos(tw)\ \mathrm{d}w\\ &=\frac{\pi}{4t}\left[t\coth\left(\frac{t}{2}\right)-2\right]\mathrm{csch}\left(\frac{t}{2}\right)\\ &=\frac{\pi\cosh(t/2)}{4\sinh^2(t/2)}-\frac{\pi}{2t\sinh(t/2)}.\end{aligned} \quad \text{(C19)}$$

We can at last write $\Upsilon_1$ in the form given by Jin and Korepin [7]

$$\Upsilon_1=-\int_0^{\infty}\left[\frac{e^{-t}}{3t}+\frac{1}{t\sinh^2(t/2)}-\frac{\cosh(t/2)}{2\sinh^3(t/2)}\right]\mathrm{d}t. \quad \text{(C20)}$$

Moreover, we can integrate it numerically, yielding $\Upsilon_1\simeq 0.495018$.

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[23] However, in information and computation theory the above formulas are customarily written taking base-two logarithms.

[24] Naively it could be thought that a spinless fermion would violate the spin-statistics theorem; however, as we are not considering a 3+1 relativistic quantum field theory, this is not the case.

[25] If indices $\alpha_i$ and $\beta_j$ are arbitrary, placing the operators in the order appearing on the right-hand side of Eq. (39) could lead to some minus sign, since $g_i^{(\dagger)}$ anticonmmutes with $g_j^{(\dagger)}$ if $i \neq j$, and hence we have included a "±" sign. However, once they are ordered this way, the resulting product is zero if $\alpha_i \neq \beta_i$ for some $i$. If,

oppositely, $\alpha_i = \beta_i$ for every $i$, then we have to permute the combination $O_i^{\alpha_i \dagger} O_i^{\alpha_i}$, which commutes with every operator at sites $j \neq i$ since it has an even number of operators $g_i$ or $g_i^\dagger$.

[26] Most algorithms for eigenvalue decomposition have the complexity of matrix multiplication, i.e. multiplying the $L$ elements of a row for the $L$ rows and the $L$ columns.

[27] Note that Eq. (54) is just the dominant term of the asymptotic approximation. Indeed, the complete approximation is given by Eq. (57), and clearly the ratio between its second term, $-(1-x)\log(1-x)$, and its fist term, $-x \log x$, goes to 0 as $x \to 0$. However, this ratio goes to 0 *logarithmically.* To give some numbers, let $x = 10^{-n}$, so that

$$\frac{x \log x}{(1-x)\log(1-x)} \simeq -\log x = n \log 10 \simeq 2.3n \,.$$

Then, for the values in Fig. 4 ($p_c \simeq 10^{-5}$ and $L \sim 30$), we have $x \sim 10 \cdot 10^{-5} = 10^{-4}$, and thus $2.3n \simeq 9.2$; i.e., the second term is more than 10% of the first one, which is small but appreciable.

[28] We remark that the correspondence of being critical (resp. gapped) and having a logarithmically divergent (resp. saturing) entropy holds true for local systems only. There exist gapped models with long-range interactions and a fractal structure of the Fermi surface that obey a volume law rather than an area law [3].

[29] Actually, every Rényi entanglement entropy must behave like the one of a CFT, and not even this far more restrictive condition is sufficient.

[30] Actually, there is a difference, since the dispersion relation (the $\Lambda_k$ factor in Eq. (17)) changes for each system, and determines $p_c$ through the relation $p_c = 2\pi k_c/N$ with $\Lambda_k|_{k_c} = 0$. In other words, $p_c$ is the value of the momentum corresponding to the (approx.) integer $k_c$ from which $\Lambda_k$ becomes positive, and therefore the modes with $k_c < k \leq N - k_c$ have to be excluded. The asymptotic behaviour of the entanglement entropy for an arbitrary system of free fermions with translation invariance, whose Hamiltonian is of the form (12), is then given by $S_L \simeq \frac{1}{3}\log(2\mathcal{L}) + \Upsilon_1$, with $\mathcal{L} = L \sin p_c$. Let us remark that the constant $\Upsilon_1$ does not depend on the model, that is, the dependence of the asymptotic formula on the model is entirely contained in $\mathcal{L}$. (The not universal character of the constant emerges when comparing the XX chain with other critical models, where the additive constant in $S_L$ is not necessarily $1/3\log(2\sin p_c) + \Upsilon_1$.)