Partial transpose of two disjoint blocks in XY spin chains

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Abstract. We consider the partial transpose of the spin reduced density matrix of two disjoint blocks in spin chains admitting a representation in terms of free fermions, such as XY chains. We exploit the solution of the model in terms of Majorana fermions and show that such partial transpose in the spin variables is a linear combination of four Gaussian fermionic operators. This representation allows to explicitly construct and evaluate the integer moments of the partial transpose. We numerically study critical XX and Ising chains and we show that the asymptotic results for large blocks agree with conformal field theory predictions if corrections to the scaling are properly taken into account.

1. Introduction

In the last decade, the understanding of the entanglement content of extended quantum systems boosted an intense research activity at the boundary between condensed matter, quantum information and quantum field theory (see e.g. Refs. [1] as reviews). The bipartite entanglement for an extended system in a pure state is measured by the well-known entanglement entropy which is the von Neumann entropy corresponding to the reduced density matrix of one of the two parts. One of the most remarkable results in this field is the logarithmic divergence of the entanglement with the subsystem size in the case when the low energy properties of the extended critical quantum systems are described by a 1+1 dimensional conformal invariant theory [2, 3, 4, 5].

Conversely, when an extended quantum system is in a mixed state (or one considers a tripartition of a pure state and is interested in the relative entanglement between two of the three parts) the quantification of the entanglement is much more complicated. A very useful concept is that of partial transposition. Indeed it has been shown that the presence of entanglement in a bipartite mixed state is related to occurrence of negative eigenvalues in the spectrum of the partial transpose of the density matrix [6]. This led to the proposal of the negativity [7] (or the logarithmic negativity) which was later shown to be an entanglement monotone [8], i.e. a good entanglement measure from a quantum information perspective. Compared to other entanglement measurements for mixed states, the negativity has the important property of being easily calculable for an arbitrary quantum state once its density matrix is known (and indeed for this reason it has been named a "computable measure of entanglement" [7]).

Recently, a systematic path integral approach to construct the partial transpose of the reduced density matrix has been developed and from this the negativity in 1+1 dimensional relativistic quantum field theories is obtained via a replica trick [9]. This approach has been successfully applied to the study of one-dimensional conformal field theories (CFT) in the ground state [9, 10], in thermal state [11, 12], and in non-equilibrium protocols [12, 13, 14, 15], as well as to topological systems [16, 17]. The CFT predictions have been tested for several models [10, 11, 13, 18, 19, 20], especially against exact results [10, 11, 13, 21] for free bosonic systems (such as the harmonic chain). Indeed for free bosonic models, the partial transposition corresponds to a time-reversal operation leading to a partially transposed reduced density matrix which is Gaussian [22] and that can be straightforwardly diagonalised by correlation matrix techniques [23, 24, 25]. It should be also mentioned that there exist some earlier results for the negativity in many body systems [21, 22, 24, 26, 27, 28, 29, 30, 31].

In the case of free fermionic systems (such as the tight-binding model and XY spin chains) the calculation of the negativity is instead much more involved. Indeed the partial transpose of the reduced density matrix is not a Gaussian operator and standard techniques based on the correlation matrix [25] cannot be applied. In view of the importance that exact calculations for free fermionic systems played in the understanding of the entanglement entropy [3, 32, 33, 34, 35, 36], it is highly desirable to have an exact representation of the negativity also for free fermionic systems. A major step in this direction has been very recently achieved by Eisler and Zimboras [37] who showed that the partial transpose is a linear combination of two Gaussian operators. Unfortunately, it is still not possible to extract the spectrum of the partial transpose and hence the negativity, but at least one can access to integer powers of the partial transpose which are the main ingredient for the replica approach to negativity.

In Ref. [37] only truly fermionic systems have been considered and not spin chains that can be mapped to a fermionic system by means of a (non-local) Jordan-Wigner transformation. Indeed, in the very interesting case of two disjoint blocks in a spin chain the density matrix of spins and fermions are not equal [39, 40, 41] and this consequently affects also the partial transposition, as already pointed out in [37]. In this manuscript we fill this gap by giving an exact representation of the partial transpose of the reduced density matrix for two disjoint blocks in the XY spin chain and from this we calculate the traces of its integer powers. These turn out to converge to the CFT predictions in the limit of large intervals.

The manuscript is organised as follows. In Sec. 2 we describe the model and the definition of the quantities we will study. In Sec. 3 we review the results of Ref. [41] for the moments of the spin reduced density matrix of two disjoint blocks. In Sec. 4 we move to the core of this manuscript deriving an explicit representation of the partial transpose of the spin reduced density matrix as a sum of four Gaussian fermionic matrices. This allows to obtain explicit representations for the moments of the partial transpose. In Sec. 5 we use the above results to numerically calculate these moments up to $n = 5$ for the critical Ising model and XX chain and carefully compare them with CFT predictions by taking into account corrections to the scaling. In Sec. 6 we numerically evaluate and study the moments of the partial transpose for two disjoint blocks of fermions and again we compare with new CFT predictions. Finally in Sec. 7 we draw our conclusions. In appendix A we report all the CFT results which we needed in this manuscript.

2. The model and the quantities of interest

In this manuscript we consider the XY spin chains with Hamiltonian

$$H_{XY} = -\frac{1}{2}\sum_{j=1}^{L}\left(\frac{1+\gamma}{2}\,\sigma_j^x\sigma_{j+1}^x + \frac{1-\gamma}{2}\,\sigma_j^y\sigma_{j+1}^y + h\,\sigma_j^z\right), \qquad (1)$$

where σ_j^α are the Pauli matrices at the j-th site and we assume periodic boundary conditions $\sigma_{L+1}^\alpha = \sigma_1^\alpha$. For $\gamma = 1$ Eq. (1) reduces to the Hamiltonian of the Ising model in a transverse field while for $\gamma = 0$ to the one of the XX spin chain. The Hamiltonian (1) is a paradigmatic model for quantum phase transitions [38]. In fact, it depends on two parameters: the transverse magnetic field h and the anisotropy parameter γ. The system is critical for $h = 1$ and any γ with a transition that belongs to the Ising universality class. It is also critical for $\gamma = 0$ and $|h| < 1$ with a continuum limit given by a free compactified boson.

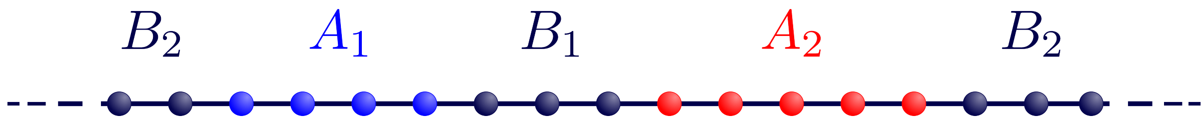

Figure 1. We consider the entanglement between two disjoint spin blocks A_1 and A_2 embedded in a spin chain of arbitrary length. The reminder of the system is denoted by B which is also composed of two disconnected pieces B_1 and B_2.

The Jordan-Wigner transformation

$$c_j = \Big(\prod_{m<j} \sigma_m^z\Big) \frac{\sigma_j^x - \mathrm{i}\sigma_j^z}{2}, \qquad c_j^\dagger = \Big(\prod_{m<j} \sigma_m^z\Big) \frac{\sigma_j^x + \mathrm{i}\sigma_j^z}{2}, \tag{2}$$

maps the spin variables into anti-commuting fermionic ones $\{c_i, c_j^\dagger\} = \delta_{ij}$. In terms of these fermionic variables the Hamiltonian (1) becomes

$$H_{XY} = \sum_{i=1}^{L} \left(\frac{1}{2} \left[\gamma c_i^\dagger c_{i+1}^\dagger + \gamma c_{i+1} c_i + c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right] - h c_i^\dagger c_i \right), \tag{3}$$

where we neglected boundary and additive terms. This Hamiltonian is quadratic in the fermionic operators and hence can be straightforwardly diagonalised in momentum space by means of a Bogoliubov transformation.

For the study of the reduced density matrices it is very useful to introduce the Majorana fermions [3]

$$a_{2j} = c_j + c_j^\dagger, \qquad a_{2j-1} = \mathrm{i}(c_j - c_j^\dagger), \tag{4}$$

which satisfy the anti-commutation relations $\{a_r, a_s\} = 2\delta_{rs}$.

2.1. Quantities of interest

The main goal of this manuscript is to determine the entanglement between two disjoint intervals in the XY spin chain. We consider the geometry depicted in Fig. 1: a spin chain is divided in two parts A and B and each of them is composed of disconnected pieces. We denote by A_1 and A_2 the two blocks in $A = A_1 \cup A_2$, B_1 is the block in B separating them, while B_2 is the remainder.

The reduced density matrix of A is $\rho_A = \mathrm{Tr}_B \rho = \mathrm{Tr}_B |\Psi\rangle\langle\Psi|$, where we are mainly interested in the case in which $|\Psi\rangle$ is the ground state of the XY chain, even if the results of this paper apply to more general cases such as excited states, non-equilibrium configurations, finite temperature etc. The bipartite entanglement between A and B is given by the well-known entanglement entropy

$$S_A = -\mathrm{Tr} \rho_A \ln \rho_A \,, \tag{5}$$

or equivalently by the Rényi entropies

$$S_A^{(n)} = \frac{1}{1-n} \ln \mathrm{Tr}\, \rho_A^n \,, \tag{6}$$

which in the limit $n \to 1$ reduce to the entanglement entropy, but provide more information since it is related to the full spectrum of ρ_A [42].

In the case of two disjoint blocks in the XY spin chain, the Rényi entropies for integer n (or equivalently the moments of the reduced density matrix ρ_A) have been explicitly constructed in Ref. [41]. However it is still not possible to find the analytic continuation to arbitrary complex values of n and consequently the entanglement entropy. This is very similar to the CFT counterpart where also one can calculate only integer moments of the reduced density matrices (see Appendix A for a summary of the CFT results of interest for this paper).

However, we are here interested in the entanglement between A_1 and A_2. A measure of this entanglement is provided by the logarithmic negativity defined as follows. Let us denote by $|e_i^{(1)}\rangle$ and $|e_j^{(2)}\rangle$ two arbitrary bases in the Hilbert spaces corresponding to A_1 and A_2. The partial transpose of ρ_A with respect to A_2 degrees of freedom is defined as

$$\langle e_i^{(1)} e_j^{(2)} | \rho_A^{T_2} | e_k^{(1)} e_l^{(2)} \rangle = \langle e_i^{(1)} e_l^{(2)} | \rho_A | e_k^{(1)} e_j^{(2)} \rangle, \tag{7}$$

and then the *logarithmic* negativity as

$$\mathcal{E} \equiv \ln ||\rho_A^{T_2}|| = \ln \mathrm{Tr}|\rho_A^{T_2}|\,, \tag{8}$$

where the trace norm $||\rho_A^{T_2}||$ is the sum of the absolute values of the eigenvalues of $\rho_A^{T_2}$.

A systematic method to compute the negativity in quantum field theories has been developed in Ref. [9, 10] and it is again based on a replica trick from the integer moments of the partial transpose

$$\mathrm{Tr}(\rho_A^{T_2})^n, \tag{9}$$

which turn out to admit different analytic continuations from even and odd n (usually denoted as n_e and n_o respectively). Consequently, the logarithmic negativity is given by the replica limit

$$\mathcal{E} = \lim_{n_e \to 1} \ln \mathrm{Tr}(\rho_A^{T_2})^{n_e}, \tag{10}$$

performed on the even sequence of moments. Unfortunately, in the case of two disjoint intervals, it is very difficult to perform this analytic continuation (see Appendix A), although the integer moments $\mathrm{Tr}(\rho_A^{T_2})^n$ are known for the most relevant conformal field theories. It is however possible to extract very useful information about entanglement and about the partial transpose already from the knowledge of the moments [9, 10].

Finally, in Refs. [9, 10] the ratios

$$R_n \equiv \frac{\mathrm{Tr}(\rho_A^{T_2})^n}{\mathrm{Tr}\rho_A^n}, \tag{11}$$

have been introduced because of some cancellations (see Appendix A) and since anyhow

$$\mathcal{E} = \lim_{n_e \to 1} \ln(R_{n_e}), \tag{12}$$

given that $\mathrm{Tr}\rho_A = 1$.

3. Rényi entropies

In this section we review the results of Ref. [41], where the Rényi entropies of two disjoint blocks $A = A_1 \cup A_2$ for the XY spin chains have been computed. These results are the main ingredients to construct the integer powers of the partial transpose which will be derived in the following section. We will denote the number of spins in A_1 and A_2 with ℓ_1 and ℓ_2 respectively and the remainder of the system B contains a region separating A_1 and A_2 denoted as B_1, as pictorially depicted in Fig. 1.

In a general spin 1/2 chain the reduced density matrix $\rho_A = \mathrm{Tr}_B|\Psi\rangle\langle\Psi|$ of $A = A_1 \cup A_2$ can be computed by summing all the operators in A as follows [3]

$$\rho_A = \frac{1}{2^{\ell_1+\ell_2}} \sum_{\nu_j} \Big\langle \prod_{j\in A} \sigma_j^{\nu_j} \Big\rangle \prod_{j\in A} \sigma_j^{\nu_j}, \tag{13}$$

where j is the index labelling the lattice sites and $\nu_j \in \{0, 1, 2, 3\}$, with $\sigma^0 = \mathbf{1}$ the identity matrix and $\sigma^1 = \sigma^x$, $\sigma^2 = \sigma^y$ and $\sigma^3 = \sigma^z$ the Pauli matrices. The multipoints correlators in (13) are very difficult to compute, unless there is a representation of the state in terms of free fermions.

For the single interval case, the Jordan-Wigner string $\prod_{m<j} \sigma_m^z$ in Eq. (2) maps the first ℓ spins into the first ℓ fermions [3] so the spin and fermionic entropy are the same. In general, calculating a fermionic density matrix is very easy. Indeed by Wick theorem they assume a Gaussian form:

$$\rho_W = \frac{\exp\left(\frac{1}{4}\sum_{r,s} a_r W_{rs} a_s\right)}{\mathrm{Tr}\left[\exp\left(\frac{1}{4}\sum_{r,s} a_r W_{rs} a_s\right)\right]}\,, \tag{14}$$

with W a complex antisymmetric matrix. This density matrix is univocally identified by the correlation matrix

$$\Gamma_{rs} = \mathrm{Tr}(a_r \rho_W a_s) - \delta_{rs}, \tag{15}$$

which (in matrix form) satisfies $\Gamma = \tanh(W/2)$.

Unfortunately, the same reasoning does not apply to two disjoint blocks because the fermions in the interval B_1 separating the two blocks contribute to the spin reduced density matrix of $A_1 \cup A_2$ [39, 40, 41]. In particular, the following string of Majorana operators appears in a crucial way‡

$$P_{B_1} \equiv \prod_{j\in B_1} (\mathrm{i} a_{2j-1} a_{2j}). \tag{16}$$

Similarly, we also introduce the strings of Majorana operators P_{A_1} and P_{A_2}, defined as in Eq. (16) but taking the product over $j \in A_1$ and $j \in A_2$ respectively. These operators satisfies $P_C^{-1} = P_C$, for any $C = A_1, A_2, B_1$.

Moving back to the computation of the spin reduced density matrix (13) in terms of fermions, we first notice that, since the XY Hamiltonian commutes with $\prod_j \sigma_j^z$ (where j runs over the whole chain), only the expectation values of operators containing an even

‡ To compare with Ref. [41], set $(S_1)_{\text{there}} = (P_{A_1})_{\text{here}}$ and $(S)_{\text{there}} = (P_{B_1})_{\text{here}}$.

number of fermions are non vanishing. Thus, the numbers of fermions are either even or odd in both A_1 and A_2. This leads us to decompose the spin reduced density matrix ρ_A of $A = A_1 \cup A_2$ as [41]

$$\rho_A \,=\, \rho_{\text{even}} + P_{B_1}\,\rho_{\text{odd}}, \tag{17}$$

with

$$\rho_{\text{even}} \equiv \frac{1}{2^{\ell_1+\ell_2}} \sum_{\text{even}} \langle O_1 O_2 \rangle\, O_2^\dagger O_1^\dagger, \qquad \rho_{\text{odd}} \equiv \frac{1}{2^{\ell_1+\ell_2}} \sum_{\text{odd}} \langle O_1 P_{B_1} O_2 \rangle\, O_2^\dagger O_1^\dagger, \tag{18}$$

where we introduced the 'shorts' O_1 and O_2 for arbitrary products of Majorana fermions in A_1 and A_2 respectively, and the notation $\sum_{\text{even}}$ ($\sum_{\text{odd}}$) means that the sum is restricted to operators O_1 and O_2 containing an even (odd) number of fermions. It is also convenient to rewrite (17) as

$$\rho_A \,=\, \frac{\mathbf{1} + P_{B_1}}{2}\,\rho_+ + \frac{\mathbf{1} - P_{B_1}}{2}\,\rho_-, \qquad \rho_\pm \equiv \rho_{\text{even}} \pm \rho_{\text{odd}}, \tag{19}$$

where $\mathbf{1}$ is the identity matrix and $(\mathbf{1} \pm P_{B_1})/2$ are orthogonal projectors. Moreover, the matrices $\rho_\pm$ are unitary equivalent (indeed $P_{A_2}\rho_\pm P_{A_2} = \rho_\mp$) and commute with P_{B_1} because they do not contain Majorana fermions in B_1. As a consequence, we have that

$$\rho_A^n \,=\, \frac{\mathbf{1} + P_{B_1}}{2}\,\rho_+^n + \frac{\mathbf{1} - P_{B_1}}{2}\,\rho_-^n. \tag{20}$$

Taking the trace of (20) and employing that $P_{A_2}\rho_\pm P_{A_2} = \rho_\mp$, one finds

$$\text{Tr}\rho_A^n = \text{Tr}\rho_\pm^n. \tag{21}$$

The matrices $\rho_\pm$ are fermionic but they are not Gaussian, i.e. they are not proportional to the exponential of a quadratic form, as we will discuss below.

At this point we are ready to consider the ground state of the XY chain with density matrix $\rho_W = |\Psi\rangle\langle\Psi|$, whose correlation matrix Γ is given by Eq. (15). The fermionic reduced density matrix of $A = A_1 \cup A_2$ is

$$\rho_A^{\mathbf{1}} \equiv \frac{1}{2^{\ell_1+\ell_2}} \sum_{\substack{\text{even}\\ \text{odd}}} \langle O_1 O_2 \rangle\, O_2^\dagger O_1^\dagger, \tag{22}$$

where we recall that $\langle O_1 O_2 \rangle = 0$ when the numbers of fermionic operators in O_1 and O_2 have different parity. In order to take into account the effect of the string P_{B_1} defined in Eq. (16), it is useful to introduce the auxiliary density matrix

$$\rho_A^{B_1} \equiv \frac{\text{Tr}_B(P_{B_1}|\Psi\rangle\langle\Psi|)}{\langle P_{B_1}\rangle}, \tag{23}$$

in which the normalisation $\text{Tr}\rho_A^{B_1} = 1$ holds. By using that

$$P_{A_2} a_j P_{A_2} = \begin{cases} -\,a_j & j \in A_2, \\ \;\;\,a_j & j \notin A_2, \end{cases} \tag{24}$$

one finds

$$P_{A_2}\rho_A^{\mathbf{1}} P_{A_2} = \frac{1}{2^{\ell_1+\ell_2}} \sum_{\substack{\text{even}\\ \text{odd}}} (-1)^{\mu_2} \langle O_1 O_2 \rangle\, O_2^\dagger O_1^\dagger \tag{25}$$

$$= \frac{1}{2^{\ell_1+\ell_2}} \sum_{\text{even}} \langle O_1 O_2 \rangle\, O_2^\dagger O_1^\dagger - \frac{1}{2^{\ell_1+\ell_2}} \sum_{\text{odd}} \langle O_1 O_2 \rangle\, O_2^\dagger O_1^\dagger, \tag{26}$$

where μ_2 is the number of Majorana operators occurring in O_2. Then, from Eqs. (22) and (26) it is straightforward to get that the density matrices (18) become

$$\rho_{\text{even}} = \frac{\rho_A^{\mathbf{1}} + P_{A_2}\rho_A^{\mathbf{1}}P_{A_2}}{2}, \qquad \rho_{\text{odd}} = \langle P_{B_1}\rangle \, \frac{\rho_A^{B_1} - P_{A_2}\rho_A^{B_1}P_{A_2}}{2}. \tag{27}$$

Plugging (27) into (17), one finds that the spin reduced density matrix is a linear combination of four fermionic Gaussian operators. Since these operators do not commute, they cannot be diagonalised simultaneously and therefore we cannot find the eigenvalues of the spin reduced density matrix that would give the entanglement entropy. Nevertheless, $\mathrm{Tr}\rho_A^n$ for integer n can be computed through Eq. (21) by providing the product rules between the four Gaussian operators occurring in (27) in terms of the corresponding correlation matrices, that are denoted by

$$\Gamma_1 \equiv \Gamma_{\rho_A^{\mathbf{1}}}, \qquad \Gamma_2 \equiv \Gamma_{P_{A_2}\rho_A^{\mathbf{1}}P_{A_2}}, \qquad \Gamma_3 \equiv \Gamma_{\rho_A^{B_1}}, \qquad \Gamma_4 \equiv \Gamma_{P_{A_2}\rho_A^{B_1}P_{A_2}}, \tag{28}$$

where Γ_ρ is the correlation matrix of a Gaussian density matrix ρ as in Eq. (15). Obviously, Γ_1 is the fermionic correlation matrix, i.e. the one of the free fermions without the Jordan-Wigner string (studied in detail in Ref. [43]).

Following Ref. [41], we can introduce the restricted correlation matrix to two fermionic sets/blocks C and D $(\Gamma_{CD})_{rs}$ which is the correlation matrix in Eq. (15) associated to $|\Psi\rangle\langle\Psi|$ with the restriction $r \in C$ and $s \in D$. In [41] it has been shown that the matrices Γ_2, Γ_3 and Γ_4 can be written as

$$\Gamma_1 = \Gamma_{AA}, \qquad \Gamma_3 = \Gamma_1 - \Gamma_{AB_1}\Gamma^{-1}_{B_1B_1}\Gamma_{B_1A}, \tag{29}$$

and

$$\Gamma_2 = M_2\Gamma_1M_2, \qquad \Gamma_4 = M_2\Gamma_3M_2, \qquad M_2 \equiv \begin{pmatrix} \mathbf{1}_{\ell_1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1}_{\ell_2} \end{pmatrix}. \tag{30}$$

These formulas provide an explicit representation of the matrices Γ_i in terms of the fermion correlation in the finite subsystem $A_1 \cup B_1 \cup A_2$.

By introducing the following notation

$$\{\ldots, \Gamma, \ldots, \Gamma', \ldots\} \equiv \mathrm{Tr}(\ldots \rho_W \ldots \rho_{W'} \ldots), \tag{31}$$

and $\{\ldots, \Gamma^n, \ldots\} \equiv \mathrm{Tr}(\ldots \rho_W^n \ldots)$ as special case, from (27) we have that $\mathrm{Tr}\rho_\pm^n$ can be written as a linear combination of traces involving the matrices Γ_k with $k \in \{1,2,3,4\}$. This finally provides $\mathrm{Tr}\rho_A^n$, which we write as follows

$$\mathrm{Tr}\rho_A^n \equiv \frac{T_n}{2^{n-1}}. \tag{32}$$

From (21) and (27), it is straightforward to realise that T_n is a combination of 4^n terms of the form (31) with coefficients given by integer powers of $\delta_{B_1} \equiv \langle P_{B_1}\rangle^2 = \det[\Gamma_{B_1B_1}]$. However, many of these 4^n terms turn out to be equal when using cyclicality of the trace and other simple algebraic manipulations.

In the following we write T_n explicitly for $2 \leqslant n \leqslant 5$, where we have computed also T_5, in addition to the other ones already reported in Ref. [41]:

• $n = 2$:

$$T_2 \;=\; \{\Gamma_1^2\} + \{\Gamma_1, \Gamma_2\} + \delta_{B_1}\Big(\{\Gamma_3^2\} - \{\Gamma_3, \Gamma_4\}\Big); \tag{33}$$

• $n = 3$:

$$T_3 = \{\Gamma_1^3\} + 3\{\Gamma_1^2, \Gamma_2\} + 3\delta_{B_1}\Big(\{\Gamma_1, \Gamma_3^2\} + \{\Gamma_2, \Gamma_3^2\} - 2\{\Gamma_1, \Gamma_4, \Gamma_3\}\Big); \quad (34)$$

• $n = 4$:

$$\begin{aligned} T_4 = \ & \{\Gamma_1^4\} + \{\Gamma_1, \Gamma_2, \Gamma_1, \Gamma_2\} + 4\{\Gamma_1^3, \Gamma_2\} + 2\{\Gamma_1^2, \Gamma_2^2\} \\ & + 2\delta_{B_1}\Big(\{\Gamma_1, \Gamma_3, \Gamma_1, \Gamma_3\} + \{\Gamma_1, \Gamma_4, \Gamma_1, \Gamma_4\} + 2\{\Gamma_1^2, \Gamma_3^2\} + 2\{\Gamma_1^2, \Gamma_4^2\} \\ & \qquad + 2\{\Gamma_1, \Gamma_3, \Gamma_2, \Gamma_3\} + 4\{\Gamma_1, \Gamma_2, \Gamma_3^2\} - 2[2\{\Gamma_1^2, \Gamma_3, \Gamma_4\} \\ & \qquad + \{\Gamma_1, \Gamma_3, \Gamma_1, \Gamma_4\} + \{\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4\} + \{\Gamma_1, \Gamma_3, \Gamma_2, \Gamma_4\} + \{\Gamma_1, \Gamma_2, \Gamma_4, \Gamma_3\}]\Big) \\ & + \delta_{B_1}^2\Big(\{\Gamma_3^4\} + 2\{\Gamma_3^2, \Gamma_4^2\} + \{\Gamma_3, \Gamma_4, \Gamma_3, \Gamma_4\} - 4\{\Gamma_3^3, \Gamma_4\}\Big); \end{aligned} \quad (35)$$

• $n = 5$

$$\begin{aligned} T_5 = \ & \{\Gamma_1^5\} + 5\Big(\{\Gamma_1^4, \Gamma_2\} + \{\Gamma_1^3, \Gamma_2^2\} + \{\Gamma_1^2, \Gamma_2, \Gamma_1, \Gamma_2\}\Big) \\ & + 5\delta_{B_1}\Big(\{\Gamma_1^3, \Gamma_3^2\} + \{\Gamma_1^3, \Gamma_4^2\} + 2\{\Gamma_1, \Gamma_2^2, \Gamma_3^2\} + 2\{\Gamma_1^2, \Gamma_2, \Gamma_3^2\} \\ & \quad + \{\Gamma_1, \Gamma_2, \Gamma_1, \Gamma_3^2\} + \{\Gamma_1, \Gamma_2, \Gamma_1, \Gamma_4^2\} + \{\Gamma_1^2, \Gamma_3, \Gamma_1, \Gamma_3\} + \{\Gamma_1^2, \Gamma_3, \Gamma_2, \Gamma_3\} \\ & \quad + 2\{\Gamma_1, \Gamma_3, \Gamma_1, \Gamma_3, \Gamma_2\} + \{\Gamma_1, \Gamma_3, \Gamma_2^2, \Gamma_3\} + \{\Gamma_1^2, \Gamma_4, \Gamma_1, \Gamma_4\} + 2\{\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_2, \Gamma_3\} \\ & \quad - 2[\{\Gamma_1^2, \Gamma_2, \Gamma_4, \Gamma_3\} + \{\Gamma_1^2, \Gamma_2, \Gamma_3, \Gamma_4\} + \{\Gamma_1^2, \Gamma_3, \Gamma_1, \Gamma_4\} + \{\Gamma_1^2, \Gamma_3, \Gamma_2, \Gamma_4\} \\ & \qquad + \{\Gamma_1^3, \Gamma_3, \Gamma_4\} + \{\Gamma_1, \Gamma_2, \Gamma_1, \Gamma_3, \Gamma_4\} + \{\Gamma_1, \Gamma_2, \Gamma_4, \Gamma_1, \Gamma_3\} + \{\Gamma_2, \Gamma_1, \Gamma_4, \Gamma_1, \Gamma_3\}]\Big) \\ & + 5\delta_{B_1}^2\Big(\{\Gamma_1, \Gamma_3^4\} + \{\Gamma_2, \Gamma_3^4\} + 2\{\Gamma_1, \Gamma_3^2, \Gamma_4^2\} + \{\Gamma_1, \Gamma_3, \Gamma_4^2, \Gamma_3\} + 2\{\Gamma_1, \Gamma_3, \Gamma_4, \Gamma_3, \Gamma_4\} \\ & \quad + \{\Gamma_1, \Gamma_4, \Gamma_3^2, \Gamma_4\} - 2[\{\Gamma_1, \Gamma_3^3, \Gamma_4\} + \{\Gamma_1, \Gamma_3^2, \Gamma_4, \Gamma_3\} + \{\Gamma_2, \Gamma_4, \Gamma_3^3\} + \{\Gamma_2, \Gamma_3^2, \Gamma_4, \Gamma_3\}]\Big). \end{aligned} \quad (36)$$

We notice that the algebraic sum of the integer coefficients occurring in any term multiplying a power $\delta_{B_1}^p$ with $p > 0$ is zero. Moreover, considering only the terms which are not multiplied by a power δ_{B_1} in T_n, the sum of their coefficients is 2^{n-1}.

4. Traces of integer powers of the partial transpose of the spin reduced density matrix

In this section we move to the main objective of this paper which is to give a representation of the integer powers of the partial transpose of the spin reduced density matrix of two disjoint blocks with respect to A_2. Eisler and Zimboras in Ref. [37] showed how to obtain the partial transpose of a fermionic Gaussian density matrix, a procedure which can be applied to the spin reduced density matrix in Eq. (19) using the linearity of the partial transpose as we are going to show. We mention that in Ref. [37] the moments of the partial transpose for two adjacent intervals were studied in details using the property that fermionic and spin reduced density matrices are equal for this special case.

Given a Gaussian density matrix ρ_W written in terms of Majorana fermions in $A = A_1 \cup A_2$, the partial transposition with respect to A_2 leaves invariant the modes in A_1 and acts only on the ones in A_2. Furthermore, the partial transposition with respect to A_2 of ρ_A in (17) leaves the operator P_{B_1} unchanged (because it does not contain modes in A_2), therefore we have

$$\rho_A^{T_2} \;=\; \rho_{\rm even}^{T_2} + P_{B_1}\,\rho_{\rm odd}^{T_2} \;=\; \frac{\mathbf{1}+P_{B_1}}{2}\,\rho_+^{T_2} + \frac{\mathbf{1}-P_{B_1}}{2}\,\rho_-^{T_2}, \tag{37}$$

where

$$\rho_\pm^{T_2} = \rho_{\rm even}^{T_2} \pm \rho_{\rm odd}^{T_2}, \tag{38}$$

as clear from Eq. (19) because of the linearity of the partial transpose. The partial transposition of an arbitrary product of Majorana fermions A_2 (denoted shortly as O_2 like in the previous section) is given by the following map [37]

$$\mathcal{R}_2(O_2) \equiv (-1)^{\tau(\mu_2)} O_2, \qquad \tau(\mu_2) \equiv \begin{cases} 0 & (\mu_2 \bmod 4) \in \{0,3\}, \\ 1 & (\mu_2 \bmod 4) \in \{1,2\}, \end{cases} \tag{39}$$

where we recall that μ_2 is the number of Majorana operators in O_2. Then, applying Eq. (39) to (18), we find

$$\begin{aligned} \rho_{\rm even}^{T_2} &= \frac{1}{2^{\ell_1+\ell_2}} \sum_{\rm even} (-1)^{\mu_2/2} \langle O_1 O_2\rangle\, O_2^\dagger O_1^\dagger, \\ \rho_{\rm odd}^{T_2} &= \frac{1}{2^{\ell_1+\ell_2}} \sum_{\rm odd} (-1)^{(\mu_2-1)/2} \langle O_1 P_{B_1} O_2\rangle\, O_2^\dagger O_1^\dagger, \end{aligned} \tag{40}$$

which gives the desired fermionic representation of the partial transpose of the spin reduced density matrix.

At this point the moments of $\rho_A^{T_2}$ can be obtained following the same reasoning as for the moments of ρ_A. Indeed, since $\rho_\pm^{T_2}$ are unitarily equivalent ($P_{A_2}\rho_\pm^{T_2}P_{A_2} = \rho_\mp^{T_2}$ because $P_{A_2}\rho_{\rm even}^{T_2}P_{A_2} = \rho_{\rm even}^{T_2}$ and $P_{A_2}\rho_{\rm odd}^{T_2}P_{A_2} = -\rho_{\rm odd}^{T_2}$) and P_{B_1} commutes with them, starting from (37) and repeating the same observations that lead to (21), one gets

$$\mathrm{Tr}(\rho_A^{T_2})^n = \mathrm{Tr}(\rho_\pm^{T_2})^n. \tag{41}$$

Similarly to the case of the Rényi entropies considered in Sec. 3 (see Eq. (21)), the matrices $\rho_\pm^{T_2}$ are fermionic but not Gaussian. In the following we write them as sums of four Gaussian matrices, as done in (17) and (27) for ρ_A. In particular, by introducing

$$\tilde\rho_A^{\mathbf{1}} \equiv \frac{1}{2^{\ell_1+\ell_2}} \sum_{\substack{\rm even\\ \rm odd}} \mathrm{i}^{\mu_2} \langle O_1 O_2\rangle\, O_2^\dagger O_1^\dagger, \qquad \tilde\rho_A^{B_1} \equiv \frac{1}{2^{\ell_1+\ell_2}} \sum_{\substack{\rm even\\ \rm odd}} \mathrm{i}^{\mu_2}\, \frac{\langle O_1 P_{B_1} O_2\rangle}{\langle P_{B_1}\rangle}\, O_2^\dagger O_1^\dagger, \tag{42}$$

one has that the matrices in (40) become

$$\rho_{\rm even}^{T_2} = \frac{\tilde\rho_A^{\mathbf{1}} + P_{A_2}\tilde\rho_A^{\mathbf{1}}P_{A_2}}{2}, \qquad \rho_{\rm odd}^{T_2} = \langle P_{B_1}\rangle\, \frac{\tilde\rho_A^{B_1} - P_{A_2}\tilde\rho_A^{B_1}P_{A_2}}{2\mathrm{i}}, \tag{43}$$

telling us that $\rho_\pm^{T_2}$ in (38) are linear combinations of four Gaussian fermionic matrices occurring in the r.h.s.'s of (43). Notice that $\rho_{\rm even}^{T_2}$ and $\rho_{\rm odd}^{T_2}$ are Hermitian but the matrices defining them are not since

$$(\tilde\rho_A^{\mathbf{1}})^\dagger = P_{A_2}\tilde\rho_A^{\mathbf{1}}P_{A_2}, \qquad (\tilde\rho_A^{B_1})^\dagger = P_{A_2}\tilde\rho_A^{B_1}P_{A_2}. \tag{44}$$

In order to compute the correlation matrices associated to the four matrices in Eq. (43), it is convenient to introduce

$$\widetilde{M}_2 \equiv \begin{pmatrix} \mathbf{1}_{\ell_1} & \mathbf{0} \\ \mathbf{0} & \mathrm{i}\mathbf{1}_{\ell_2} \end{pmatrix}. \tag{45}$$

Then, the correlation matrices associated to $\tilde{\rho}_A^{\mathbf{1}}$, $P_{A_2}\tilde{\rho}_A^{\mathbf{1}}P_{A_2}$, $\tilde{\rho}_A^{B_1}$ and $P_{A_2}\tilde{\rho}_A^{B_1}P_{A_2}$ are given by

$$\widetilde{\Gamma}_k \equiv \widetilde{M}_2 \Gamma_k \widetilde{M}_2, \qquad k \in \{1,2,3,4\}. \tag{46}$$

In analogy to Eq. (32), we write the moments of $\rho_A^{T_2}$ as

$$\mathrm{Tr}(\rho_A^{T_2})^n = \frac{\widetilde{T}_n}{2^{n-1}}. \tag{47}$$

From Eqs. (38), (41) and (43), we have that $\widetilde{T}_n$ is a linear combination of 4^n terms. The net effect is that $\widetilde{T}_n$ can be written by taking T_n and replacing Γ_i with $\widetilde{\Gamma}_i$ and δ_{B_1} with $-\delta_{B_1}$. The latter rule comes from the imaginary unit in the denominator of $\rho_{\mathrm{odd}}^{T_2}$ in Eq. (43).

In the following we write explicitly $\widetilde{T}_n$ for $2 \leqslant n \leqslant 5$:

- $n = 2$

$$\widetilde{T}_2 = \{\widetilde{\Gamma}_1^2\} + \{\widetilde{\Gamma}_1,\widetilde{\Gamma}_2\} + \delta_{B_1}\Big(\{\widetilde{\Gamma}_3,\widetilde{\Gamma}_4\} - \{\widetilde{\Gamma}_3^2\}\Big); \tag{48}$$

- $n = 3$

$$\widetilde{T}_3 = \{\widetilde{\Gamma}_1^3\} + 3\,\{\widetilde{\Gamma}_1^2,\widetilde{\Gamma}_2\} + 3\delta_{B_1}\Big(2\,\{\widetilde{\Gamma}_1,\widetilde{\Gamma}_4,\widetilde{\Gamma}_3\} - \{\widetilde{\Gamma}_1,\widetilde{\Gamma}_3^2\} - \{\widetilde{\Gamma}_2,\widetilde{\Gamma}_3^2\}\Big); \tag{49}$$

- $n = 4$

$$\begin{aligned}\widetilde{T}_4 = {} & \{\widetilde{\Gamma}_1^4\} + \{\widetilde{\Gamma}_1,\widetilde{\Gamma}_2,\widetilde{\Gamma}_1,\widetilde{\Gamma}_2\} + 4\,\{\widetilde{\Gamma}_1^3,\widetilde{\Gamma}_2\} + 2\,\{\widetilde{\Gamma}_1^2,\widetilde{\Gamma}_2^2\} \\ & + 2\delta_{B_1}\Big(2\,\{\widetilde{\Gamma}_3,\widetilde{\Gamma}_1,\widetilde{\Gamma}_4,\widetilde{\Gamma}_1\} + 2\,\{\widetilde{\Gamma}_1,\widetilde{\Gamma}_2,\widetilde{\Gamma}_3,\widetilde{\Gamma}_4\} + 2\,\{\widetilde{\Gamma}_1,\widetilde{\Gamma}_3,\widetilde{\Gamma}_2,\widetilde{\Gamma}_4\} + 2\,\{\widetilde{\Gamma}_1,\widetilde{\Gamma}_2,\widetilde{\Gamma}_4,\widetilde{\Gamma}_3\} \\ & \qquad + 4\,\{\widetilde{\Gamma}_3,\widetilde{\Gamma}_4,\widetilde{\Gamma}_1^2\} - 2\,\{\widetilde{\Gamma}_1,\widetilde{\Gamma}_3,\widetilde{\Gamma}_2,\widetilde{\Gamma}_3\} - 4\,\{\widetilde{\Gamma}_1,\widetilde{\Gamma}_2,\widetilde{\Gamma}_3^2\} \\ & \qquad - \{\widetilde{\Gamma}_1,\widetilde{\Gamma}_3,\widetilde{\Gamma}_1,\widetilde{\Gamma}_3\} - \{\widetilde{\Gamma}_1,\widetilde{\Gamma}_4,\widetilde{\Gamma}_1,\widetilde{\Gamma}_4\} - 2\,\{\widetilde{\Gamma}_1^2,\widetilde{\Gamma}_3^2\} - 2\,\{\widetilde{\Gamma}_1^2,\widetilde{\Gamma}_4^2\}\Big) \\ & + \delta_{B_1}^2\,\Big(\{\widetilde{\Gamma}_3^4\} + 2\,\{\widetilde{\Gamma}_3^2,\widetilde{\Gamma}_4^2\} + \{\widetilde{\Gamma}_3,\widetilde{\Gamma}_4,\widetilde{\Gamma}_3,\widetilde{\Gamma}_4\} - 4\,\{\widetilde{\Gamma}_3^3,\widetilde{\Gamma}_4\}\Big)\,;\end{aligned} \tag{50}$$

- $n = 5$

$$\begin{aligned}\widetilde{T}_5 = {} & \{\widetilde{\Gamma}_1^5\} + 5\Big(\{\widetilde{\Gamma}_1^4,\widetilde{\Gamma}_2\} + \{\widetilde{\Gamma}_1^3,\widetilde{\Gamma}_2^2\} + \{\widetilde{\Gamma}_1^2,\widetilde{\Gamma}_2,\widetilde{\Gamma}_1,\widetilde{\Gamma}_2\}\Big) \\ & + 5\delta_{B_1}\Big(2\,\{\widetilde{\Gamma}_1^2,\widetilde{\Gamma}_2,\widetilde{\Gamma}_4,\widetilde{\Gamma}_3\} + 2\,\{\widetilde{\Gamma}_1^2,\widetilde{\Gamma}_2,\widetilde{\Gamma}_3,\widetilde{\Gamma}_4\} + 2\,\{\widetilde{\Gamma}_1^2,\widetilde{\Gamma}_3,\widetilde{\Gamma}_1,\widetilde{\Gamma}_4\} + 2\,\{\widetilde{\Gamma}_1^2,\widetilde{\Gamma}_3,\widetilde{\Gamma}_2,\widetilde{\Gamma}_4\} \\ & \quad + 2\,\{\widetilde{\Gamma}_1^3,\widetilde{\Gamma}_3,\widetilde{\Gamma}_4\} + 2\,\{\widetilde{\Gamma}_1,\widetilde{\Gamma}_2,\widetilde{\Gamma}_1,\widetilde{\Gamma}_3,\widetilde{\Gamma}_4\} + 2\,\{\widetilde{\Gamma}_1,\widetilde{\Gamma}_2,\widetilde{\Gamma}_4,\widetilde{\Gamma}_1,\widetilde{\Gamma}_3\} + 2\,\{\widetilde{\Gamma}_1,\widetilde{\Gamma}_4,\widetilde{\Gamma}_1,\widetilde{\Gamma}_3,\widetilde{\Gamma}_2\} \\ & \quad - \{\widetilde{\Gamma}_1^3,\widetilde{\Gamma}_3^2\} - \{\widetilde{\Gamma}_1^3,\widetilde{\Gamma}_4^2\} - 2\,\{\widetilde{\Gamma}_1,\widetilde{\Gamma}_2^2,\widetilde{\Gamma}_3^2\} - 2\,\{\widetilde{\Gamma}_1^2,\widetilde{\Gamma}_2,\widetilde{\Gamma}_3^2\} \\ & \quad - \{\widetilde{\Gamma}_1,\widetilde{\Gamma}_2,\widetilde{\Gamma}_1,\widetilde{\Gamma}_3^2\} - \{\widetilde{\Gamma}_1,\widetilde{\Gamma}_2,\widetilde{\Gamma}_1,\widetilde{\Gamma}_4^2\} - \{\widetilde{\Gamma}_1^2,\widetilde{\Gamma}_3,\widetilde{\Gamma}_1,\widetilde{\Gamma}_3\} - \{\widetilde{\Gamma}_1^2,\widetilde{\Gamma}_3,\widetilde{\Gamma}_2,\widetilde{\Gamma}_3\} \\ & \quad - 2\,\{\widetilde{\Gamma}_1,\widetilde{\Gamma}_3,\widetilde{\Gamma}_1,\widetilde{\Gamma}_3,\widetilde{\Gamma}_2\} - \{\widetilde{\Gamma}_1,\widetilde{\Gamma}_3,\widetilde{\Gamma}_2^2,\widetilde{\Gamma}_3\} - \{\widetilde{\Gamma}_1^2,\widetilde{\Gamma}_4,\widetilde{\Gamma}_1,\widetilde{\Gamma}_4\} - 2\,\{\widetilde{\Gamma}_1,\widetilde{\Gamma}_2,\widetilde{\Gamma}_3,\widetilde{\Gamma}_2,\widetilde{\Gamma}_3\}\Big) \\ & + 5\delta_{B_1}^2\,\Big(\{\widetilde{\Gamma}_1,\widetilde{\Gamma}_3^4\} + \{\widetilde{\Gamma}_2,\widetilde{\Gamma}_3^4\} + \{\widetilde{\Gamma}_1,\widetilde{\Gamma}_3,\widetilde{\Gamma}_4^2,\widetilde{\Gamma}_3\} + \{\widetilde{\Gamma}_1,\widetilde{\Gamma}_4,\widetilde{\Gamma}_3^2,\widetilde{\Gamma}_4\} + 2\,\{\widetilde{\Gamma}_1,\widetilde{\Gamma}_3,\widetilde{\Gamma}_4,\widetilde{\Gamma}_3,\widetilde{\Gamma}_4\} \\ & + 2\,\{\widetilde{\Gamma}_1,\widetilde{\Gamma}_3^2,\widetilde{\Gamma}_4^2\} - 2\,\{\widetilde{\Gamma}_1,\widetilde{\Gamma}_3^3,\widetilde{\Gamma}_4\} - 2\,\{\widetilde{\Gamma}_1,\widetilde{\Gamma}_3^2,\widetilde{\Gamma}_4,\widetilde{\Gamma}_3\} - 2\,\{\widetilde{\Gamma}_2,\widetilde{\Gamma}_4,\widetilde{\Gamma}_3^3\} - 2\,\{\widetilde{\Gamma}_2,\widetilde{\Gamma}_3^2,\widetilde{\Gamma}_4,\widetilde{\Gamma}_3\}\Big).\end{aligned} \tag{51}$$

As for T_n, also in $\widetilde{T}_n$ the algebraic sum of the integer coefficients occurring in any term multiplying a power $\delta_{B_1}^p$ with $p > 0$ vanishes.

5. Numerical results for the ground state of the critical Ising and XX model

The results of the previous section for the moments of the partial transpose of the reduced density matrix of two disjoint blocks are valid for arbitrary configurations of the XY spin chain: equilibrium, non-equilibrium, finite and infinite systems, critical and non-critical values of the parameters γ and h. In this section we evaluate numerically these moments for the configurations that so far attracted most of the theoretical interest, namely the critical points of the XY Hamiltonian, whose scaling properties are described by conformal field theories. A great advantage of the present approach compared to purely numerical methods such as exact diagonalization or tensor networks techniques is that it allows to deal directly with infinite chains without any approximations, reducing the systematic errors in the estimates of asymptotic results. Indeed, all the numerical results presented in the following are obtained for infinite chains.

We will consider two particular points of the XY Hamiltonian, namely the critical Ising model for $\gamma = h = 1$ and the zero field XX spin chain (corresponding to fermions at half-filling) obtained for $\gamma = h = 0$. The scaling limit of the former is the Ising CFT with central charge $c = 1/2$, while the scaling limit of the latter is a compactified boson at the Dirac point with $c = 1$.

The CFT predictions for the moments of both reduced density matrix and its partial transpose have been derived in a series of manuscripts and they are reviewed in Appendix A. For both models we consider the case of two disjoint blocks of equal length ℓ embedded in an infinite chain and placed at distance r. We numerically evaluate the moments of ρ_A and $\rho_A^{T_2}$ using the trace formulas of the previous sections for $n = 2, 3, 4, 5$ and we compute the ratio R_n (defined in Eq. (11)):

$$R_n \equiv \frac{\mathrm{Tr}(\rho_A^{T_2})^n}{\mathrm{Tr}\rho_A^n}, \tag{52}$$

whose (unknown) analytic continuation for $n_e \to 1$ would give the negativity. Notice that from Eqs. (32) and (47) we have that $R_n = \widetilde{T}_n/T_n$. In the scaling limit (i.e. $\ell, r \to \infty$ with ratio fixed) the ratio R_n converges to the CFT prediction (cf. Eq. (81) in Appendix) written in terms of the four-point ratio x, which is

$$x = \left(\frac{\ell}{\ell + r}\right)^2, \tag{53}$$

when specialised to the case of two intervals of equal length ℓ at distance r.

5.1. The critical Ising chain

The negativity and the moments of $\rho_A^{T_2}$ for the critical Ising chain in a transverse field have been already numerically considered in Ref. [18] by using a tree tensor network algorithm and in Ref. [19] by Monte Carlo simulations of the two-dimensional classical

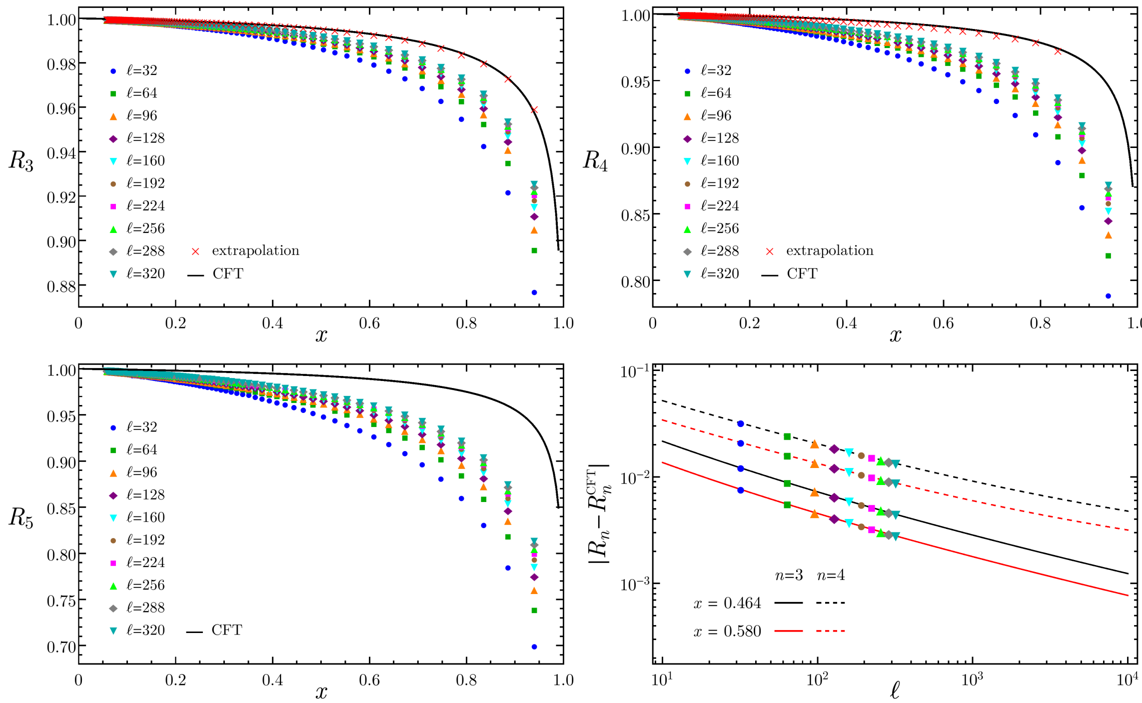

Figure 2. The ratio R_n between the integer moments of ρ_A and $\rho_A^{T_2}$ for two disjoint blocks of length ℓ at distance r embedded in an infinite critical Ising chain. We report the results for $n = 3, 4, 5$ as function of the four-point ratio x for various values of ℓ (and correspondingly of r). For large ℓ, the data approach the CFT predictions (solid lines). The extrapolations to $\ell \to \infty$ –done using the scaling form (54)– are shown as crosses and they perfectly agree with the CFT curves for $n = 3$ and 4, while for $n = 5$ the fits are unstable and the extrapolations are not shown. The last panel shows explicitly the extrapolating functions for two values of x and $n = 3, 4$.

problem in the same universality class. However, the finiteness of the chain length did not allow to obtain very precise extrapolations to the scaling theory for all values of n and of the four-point ratio x. We found, as generally proved [9], that R_2 is identically equal to 1. In Fig. 2 we report the obtained values of R_n for $n = 3, 4, 5$ as function of x for different values of ℓ. It is evident that increasing ℓ the data approach the CFT predictions (the solid curves). We can also perform an accurate scaling analysis to show that indeed the data converge to the CFT results when the corrections to the scaling are properly taken into account.

It has been argued on the basis of the general CFT arguments [44], and shown explicitly in few examples [35, 45, 46] both analytically and numerically, that $\mathrm{Tr}\rho_A^n$ displays 'unusual' corrections to the scaling which, at the leading order, are governed by the unusual exponent $\delta_n = 2h/n$ where h is the smallest scaling dimension of a relevant operator which is inserted locally at the branch point [44]. For the Ising model it has been found that, in the case of two intervals, $h = 1/2$ [39, 41]. From the general CFT arguments in Ref. [44], we expect the same corrections to be present for $\mathrm{Tr}(\rho_A^{T_2})^n$ because they are only due to the conical singularities. Unfortunately, the corrections to the scaling in Fig. 2 cannot be captured by a single term, because subleading corrections become more and more important when n increases, as already pointed out in Ref. [18]. Indeed, corrections of the form $\ell^{-m/n}$ for any integer m are know to be present [35, 41, 57]. Thus the most general finite-ℓ ansatz is of the form

$$R_n = R_n^{\rm CFT}(x) + \frac{r_n^{(1)}(x)}{\ell^{1/n}} + \frac{r_n^{(2)}(x)}{\ell^{2/n}} + \frac{r_n^{(3)}(x)}{\ell^{3/n}} + \cdots . \tag{54}$$

The variables $r_n(x)$ are used as fitting parameters in the extrapolation procedure. The number of terms that we should keep in order to have a stable fit depends both on n and on x. For each case we keep a number of terms such that the extrapolated value at $\ell \to \infty$ is stable. In any case we never keep corrections beyond the order $O(\ell^{-1})$. The results of this extrapolation procedure for $n = 3$ and 4 are explicitly reported in Fig. 2. The agreement of the extrapolations with the CFT predictions is really excellent, at an unprecedented precision compared with fully numerical computations [18, 19]. Conversely, we find that for $n = 5$ the extrapolations are still unstable because of the large number of terms we should keep in order to have a precise enough extrapolation.

5.2. The XX chain

We now move to the study of the powers of $\rho_A^{T_2}$ for the XX model in zero field. There are no previous numerical studies of this paradigmatic model. We again consider the ratios R_n for $n = 2, 3, 4, 5$ and we again find that R_2 is identically equal to 1, as it should be. In Fig. 3 we report the obtained values of R_n for $n = 3, 4, 5$ as function of x for different values of ℓ. It is evident that increasing ℓ the data approach the CFT predictions (the solid curves). We should however mention a very remarkable property. It has been observed that ${\rm Tr}\rho_A^n$ shows oscillating corrections to the scaling [35, 45, 41], which for zero magnetic field, are of the form $(-1)^\ell$. These oscillations however cancel in the ratio R_n and the corrections to the scaling are monotonous, a property which makes the extrapolation to infinite ℓ slightly simpler.

Also in this case we can perform an accurate scaling analysis to show how the data converge to the CFT results when the corrections to the scaling are properly taken into account. For the XX model, the leading correction to the scaling is governed by an exponent $\delta_n = 2/n$, which means that they are less severe than in the case of the Ising model as it is also qualitatively clear from the figure. We then use the general finite-ℓ ansatz

$$R_n = R_n^{\rm CFT}(x) + \frac{r_n^{(1)}(x)}{\ell^{2/n}} + \frac{r_n^{(2)}(x)}{\ell^{4/n}} + \frac{r_n^{(3)}(x)}{\ell^{6/n}} + \cdots , \tag{55}$$

and, as in the case of the Ising model, we keep a number of fitting parameters which make stable the extrapolation at $\ell \to \infty$. The results of this procedure for $n = 3$ and 4 are explicitly reported in Fig. 3. The agreement of the extrapolations with the CFT predictions is excellent. Also for the XX chain we find that for $n = 5$ the fits are unstable.

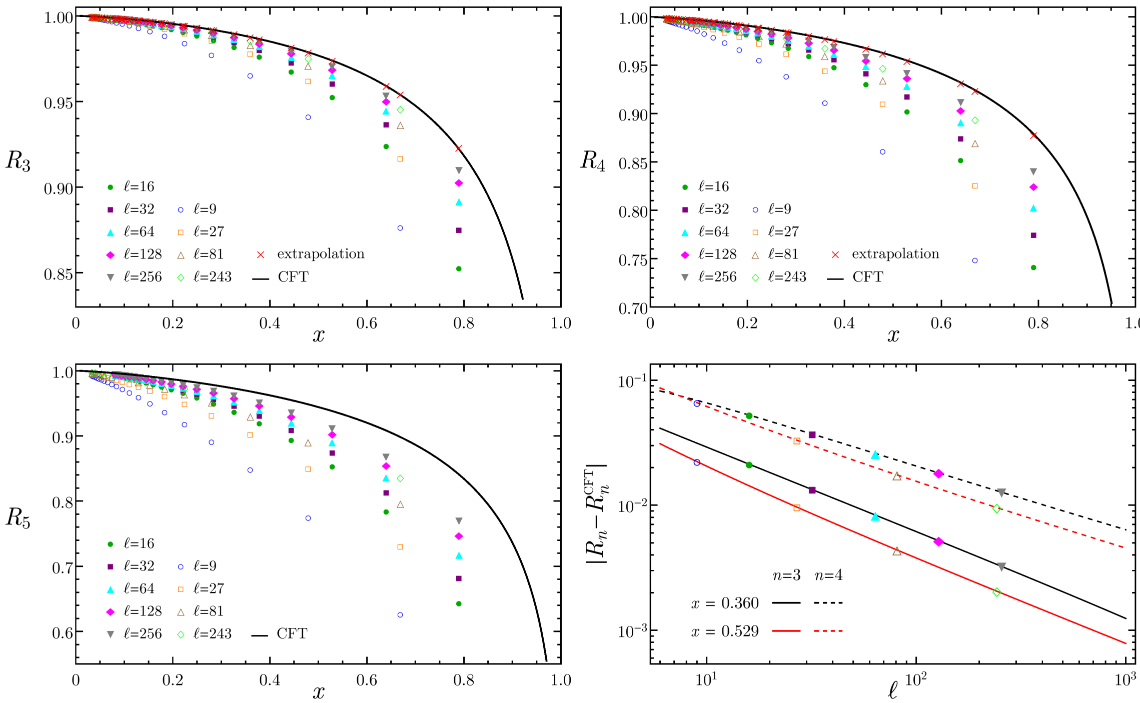

Figure 3. The ratio R_n between the integer moments of ρ_A and $\rho_A^{T_2}$ for two disjoint blocks of length ℓ at distance r embedded in an infinite XX chain at zero field. We report the results for $n = 3, 4, 5$ as function of the four-point ratio x for various values of ℓ (and correspondingly of r). For large ℓ, the data approach the CFT predictions (solid lines). The extrapolations to $\ell \to \infty$ –done using the scaling form (55)– are shown as crosses which perfectly agree with the CFT curves for $n = 3$ and 4, while for $n = 5$ the fits are unstable. The last panel shows explicitly the extrapolating functions for two values of x and $n = 3, 4$.

6. Two disjoint intervals for free fermions

In this section we consider the partial transposition for two disjoint blocks in the fermionic variables. This problem was already addressed by Eisler and Zimboras [37], but a detailed numerical analysis was not presented. For fermionic variables there is no string in B_1 connecting the two blocks (cf. Eq. (16)). Thus the partial transpose of fermions can be obtained from the formulas derived in the previous sections by discarding the string of Majorana operators (16), i.e. by replacing P_{B_1} with $\mathbf{1}$. Performing this replacement, many simplifications occur in the formulas found in Sec. 3 and Sec. 4 as we will discuss in the following.

6.1. Rényi entropies

By definition the fermionic reduced density matrix is Gaussian with correlation matrix Γ_1 defined in the Sec. 3, i.e.

$$\mathrm{Tr}\rho_A^n = \{\Gamma_1^n\}. \tag{56}$$

It is however instructive to recover this result from the formulas in Sec. 3 in order to set up the calculation for the partial transpose.

Making the replacement $P_{B_1} \to \mathbf{1}$, the reduced density matrix of the two disjoint blocks given in Eqs. (17) and (18) becomes

$$\rho_A = \rho_{\text{even}} + \rho^F_{\text{odd}}, \tag{57}$$

where§

$$\rho_{\text{even}} = \frac{1}{2^{\ell_1+\ell_2}} \sum_{\text{even}} \langle O_1 O_2 \rangle \, O_2^\dagger O_1^\dagger, \qquad \rho^F_{\text{odd}} = \frac{1}{2^{\ell_1+\ell_2}} \sum_{\text{odd}} \langle O_1 O_2 \rangle \, O_2^\dagger O_1^\dagger. \tag{58}$$

Moreover, $\rho_A^{B_1}$ defined in Eq. (23) is replaced as $\rho_A^{B_1} \to \rho_A$ and therefore, from Eqs. (27) and (57) we conclude that $\rho_+^F = \rho_A^{\mathbf{1}}$. As for the correlation matrices Γ_i, since $\rho_A^{B_1} \to \rho_A$, it is obvious that $\Gamma_3 \to \Gamma_1$ and $\Gamma_4 \to \Gamma_2$.

Summarising, we conclude that the fermionic $\mathrm{Tr}\rho_A^n$ is found by making in Eq. (32) the following replacements

$$\delta_{B_1} \to 1, \qquad \Gamma_3 \to \Gamma_1, \qquad \Gamma_4 \to \Gamma_2. \tag{59}$$

Performing these substitutions in the explicit examples given in Sec. 3 for $2 \leqslant n \leqslant 5$, it is straightforward to find Eq. (56), which is just the obvious result that the fermionic density matrix is the Gaussian operator with correlation matrix given by Γ_1.

As a further check of our numerical codes, we numerically calculated $\mathrm{Tr}\rho_A^n$ using Eq. (56) (as was already done in Ref. [43]), obtaining that on the critical lines in the scaling limit it converges to

$$\mathrm{Tr}\rho_A^n \to \frac{c_n^2}{[\ell_1 \ell_2 (1-x)]^{2\Delta_n}}, \tag{60}$$

that corresponds to $\mathcal{F}_n(x) = 1$ identically in the general CFT formula (73). Indeed this result was already proven in the continuum free fermion theory [47].

6.2. Traces of integer powers of the partial transpose

We are now ready to set up the formulas for the moments of the partial transpose, as already derived by Eisler and Zimboras [37], but numerically studied only for the case of adjacent intervals.

Once again, $\mathrm{Tr}(\rho_A^{T_2})^n$ in the fermionic variables is obtained by replacing P_{B_1} with $\mathbf{1}$ in the formulas reported in Sec. 4. Performing this replacement in Eq. (37) we get $\rho_A^{T_2} = \rho_{\text{even}}^{T_2} + (\rho^F_{\text{odd}})^{T_2} = \rho_+^{T_2}$ and in Eq. (42) it gives $\tilde\rho_A^{B_1} \to \tilde\rho_A^{\mathbf{1}}$. These observations together with Eq. (43) lead to

$$\rho_A^{T_2} = \frac{1-\mathrm{i}}{2}\,\tilde\rho_A^{\mathbf{1}} + \frac{1+\mathrm{i}}{2}\,P_{A_2}\tilde\rho_A^{\mathbf{1}}P_{A_2}, \tag{61}$$

which is exactly the same result obtained in [37] (for direct comparison, set $(O_+)_{\text{there}} = (\tilde\rho_A^{\mathbf{1}})_{\text{here}}$ and $(O_-)_{\text{there}} = (P_{A_2}\tilde\rho_A^{\mathbf{1}}P_{A_2})_{\text{here}}$).

§ To compare our notation with the one used in [37], set $(\rho_+)_{\text{there}} = (\rho_{\text{even}})_{\text{here}}$ and $(\rho_-)_{\text{there}} = (\rho^F_{\text{odd}})_{\text{here}}$.

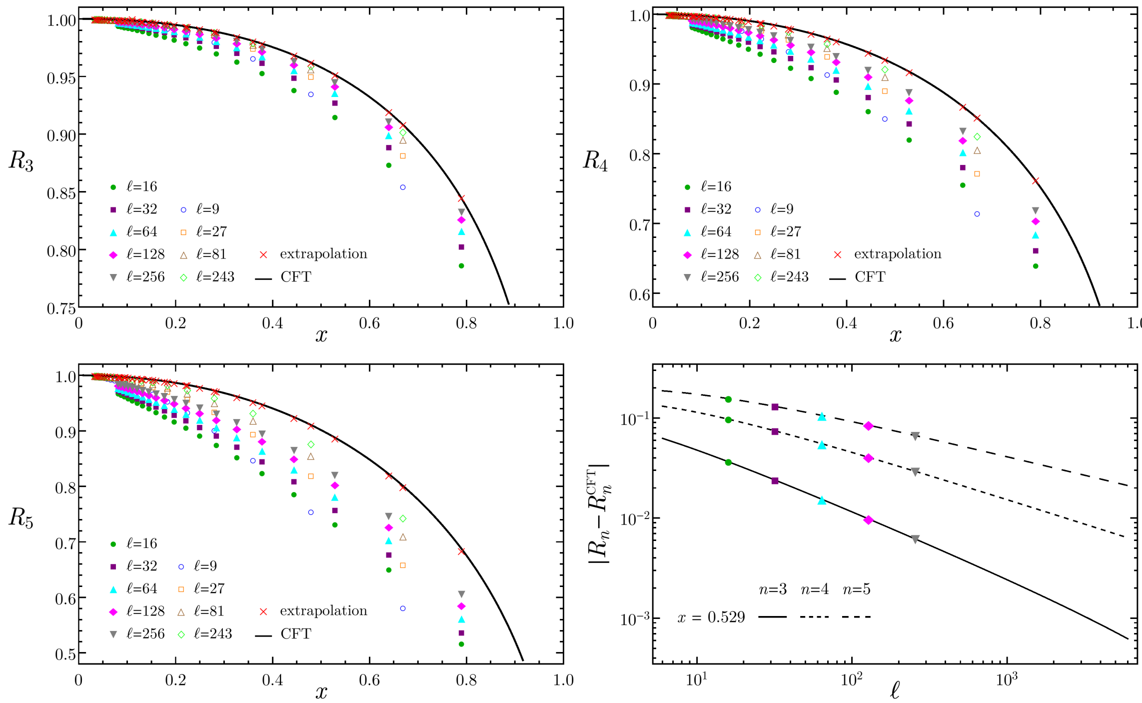

Figure 4. The ratio R_n between the integer moments of ρ_A and $\rho_A^{T_2}$ for two disjoint intervals of length ℓ at distance r for the tight-binding model at half-filling. We report the results for $n = 3, 4, 5$ as function of the four-point ratio x for various values of ℓ (and correspondingly of r). For large ℓ, the data approach the CFT predictions (solid lines). The extrapolations to $\ell \to \infty$ –done using the scaling form (55)– are shown as crosses and they perfectly agree with the CFT curves for $n = 3, 4, 5$. The last panel shows explicitly the extrapolating functions for one value of x and $n = 3, 4, 5$.

The last remaining step is just to write these formulas in terms of correlation matrices. Given that $\tilde{\rho}_A^{B_1} \to \tilde{\rho}_A^{\mathbf{1}}$, it follows that we should perform the replacements $\widetilde{\Gamma}_3 \to \widetilde{\Gamma}_1$ and $\widetilde{\Gamma}_4 \to \widetilde{\Gamma}_2$ in order to get the moments of the partial transpose in terms of the correlation matrices. Summarising, the fermionic $\mathrm{Tr}(\rho_A^{T_2})^n$ are given by the formulas in Sec. 4 performing the replacements

$$\delta_{B_1} \to 1, \qquad \widetilde{\Gamma}_3 \to \widetilde{\Gamma}_1, \qquad \widetilde{\Gamma}_4 \to \widetilde{\Gamma}_2. \tag{62}$$

Writing $\mathrm{Tr}(\rho_A^{T_2})^n = \widetilde{T}_n^F / 2^{n-1}$, and performing the replacements in the formulas for $2 \leqslant n \leqslant 5$ given in Eqs. (48), (49), (50) and (4), we find

$$\widetilde{T}_2^F = 2\,\{\widetilde{\Gamma}_1, \widetilde{\Gamma}_2\}, \tag{63}$$

$$\widetilde{T}_3^F = -2\,\{\widetilde{\Gamma}_1^3\} + 6\,\{\widetilde{\Gamma}_1^2, \widetilde{\Gamma}_2\}, \tag{64}$$

$$\widetilde{T}_4^F = -4\,\{\widetilde{\Gamma}_1^4\} + 4\,\{\widetilde{\Gamma}_1, \widetilde{\Gamma}_2, \widetilde{\Gamma}_1, \widetilde{\Gamma}_2\} + 8\,\{\widetilde{\Gamma}_1^2, \widetilde{\Gamma}_2^2\}, \tag{65}$$

$$\widetilde{T}_5^F = -4\,\{\widetilde{\Gamma}_1^5\} - 20\,\{\widetilde{\Gamma}_1^4, \widetilde{\Gamma}_2\} + 20\,\{\widetilde{\Gamma}_1^3, \widetilde{\Gamma}_2^2\} + 20\,\{\widetilde{\Gamma}_1^2, \widetilde{\Gamma}_2, \widetilde{\Gamma}_1, \widetilde{\Gamma}_2\}. \tag{66}$$

Notice that the final expressions are very compact compared to the much more cumbersome spin counterparts.

6.3. Numerical Results

We are now going to evaluate numerically the moments of the reduced density matrix and its partial transpose. We can study the problem for arbitrary values of h and γ entering in Eq. (3), but in the following we focus on the most physically relevant fermionic system with $h = \gamma = 0$, i.e. the tight binding model

$$H = \frac{1}{2}\sum_{i=1}^{L}\left[c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i\right], \tag{67}$$

at half filling ($k_F = \pi/2$). In the scaling limit, the tight binding model is described by a CFT with $c = 1$.

The numerical results for the ratios $R_n = \mathrm{Tr}(\rho_A^{T_2})^n/(\mathrm{Tr}\rho_A^n)$ are reported in Fig. 4 as function of the four-point ratio x for different ℓ and for $n = 3, 4, 5$ (we checked that $R_2 = 1$ identically, as it should). We also derived asymptotic CFT predictions for the fermionic moments of the partial transpose, but their derivation is too cumbersome and beyond the goals of this manuscript. We will report the derivation in a forthcoming publication [48] and we limit here to give the final results for $n = 2, 3, 4, 5$. In order to have manageable formulas we introduce the shorts

$$\left[\begin{array}{c} 2\boldsymbol{\varepsilon} \\ 2\boldsymbol{\delta} \end{array}\right]_\tau = \frac{|\Theta[\boldsymbol{e}](\mathbf{0}|\tau(x))|^2}{|\Theta(\mathbf{0}|\tau(x))|^2}, \tag{68}$$

where Θ is the Riemann Theta function defined in Appendix A. In terms of the Θ function the fermionic ratios R_n are given by [48]

$$\frac{2R_2}{(1-x)^{4\Delta_2}} \longrightarrow 2\left[\begin{array}{c} 0 \\ 1 \end{array}\right]_{\tilde\tau}, \tag{69}$$

$$\frac{4R_3}{(1-x)^{4\Delta_3}} \longrightarrow -2 + 6\left[\begin{array}{cc} 0 & 0 \\ 0 & 1 \end{array}\right]_{\tilde\tau}, \tag{70}$$

$$\frac{8R_4}{(1-x)^{4\Delta_4}} \longrightarrow -4 + 8\left[\begin{array}{ccc} 0 & 0 & 0 \\ 0 & 1 & 0 \end{array}\right]_{\tilde\tau} + 4\left[\begin{array}{ccc} 0 & 0 & 0 \\ 1 & 1 & 1 \end{array}\right]_{\tilde\tau}, \tag{71}$$

$$\frac{16R_5}{(1-x)^{4\Delta_5}} \longrightarrow -4 + 20\left[\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{array}\right]_{\tilde\tau} + 20\left[\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \end{array}\right]_{\tilde\tau} - 20\left[\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{array}\right]_{\tilde\tau}, \tag{72}$$

where the matrix $\tilde\tau$ has been defined in Eq. (80) and the exponent Δ_n in App. A.

It is evident from Fig. 4 that the lattice numerical results approach the CFT predictions depicted as solid lines for all n. As in the spin case, we can perform a careful finite ℓ analysis to take into account corrections to the scaling. The leading correction is expected to be of the form $\ell^{-2/n}$ and subleading ones to be integer powers of the leading one. The finite ℓ ansatz is then given by Eq. (55) and again to have an accurate description of the data we keep a number of fitting parameters which make stable the extrapolation at $\ell \to \infty$. The results of this extrapolation procedure for $n = 3, 4, 5$ are explicitly reported in Fig. 4. The agreement of the extrapolations with the CFT predictions is excellent also for $n = 5$ as a difference compared to the spin counterpart.

7. Conclusions

We have shown that the partial transpose of the reduced density matrix of two disjoint spin blocks in the XY spin chain can be written as a linear combination of four Gaussian fermionic operators, fully specified by their correlation matrices (denoted as $\widetilde{\Gamma}_i$, $i = 1, 2, 3, 4$ in the text) which have been explicitly calculated in terms of the correlation matrix of the subsystem formed by the two blocks joined with the finite part between them. This construction allows to calculate the moments of the partial transpose in generic configurations of the spin chain. In this manuscript we focused on the ground state of Ising and XY chain, but the approach is more general and can be used for arbitrary excited states, thermal density matrices, non-equilibrium situations etc.

The obtained representations of the moments of the partial transpose allow us to study in an exact manner infinite chains and very large subsystems, drastically reducing the systematic errors in the approach to the scaling limit. We found that for the ground state of the critical models the moments of the partial transpose agree (with high accuracy) with the recent CFT predictions after the corrections to the scaling are properly taken into account. We also studied numerically the integer powers of the partial transpose in the fermionic degrees of freedom (described in Ref. [37], but not numerically studied). Even in this case we find that the moments agree perfectly with the CFT predictions in [48].

The main open problem left by this manuscript for two disjoint blocks of a spin chain is whether it is somehow possible to obtain the negativity from the correlation matrix (the problem is also present for the fermionic degrees of freedom [37]). A similar problem is also open for the entanglement entropy since integer moments are obtained in a similar fashion [41], but one has no access to the spectrum of the reduced density matrix and hence to the entanglement entropy. From the practical point of view, it has been recently shown that if one knows a relative large number of integer moments, rational interpolations provide accurate estimates of the analytic continuations [49, 50] (and hence of entanglement entropy and negativity). However, a deeper understanding of these analytic continuations would be highly desirable.

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A. CFT results for entanglement entropy and negativity of two disjoint intervals

The moments of the reduced density matrix of two disjoint intervals for CFTs have been studied in a series of manuscripts [47, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63]. These results have been derived using earlier findings for the partition functions of CFTs on Riemann surfaces with non vanishing genus [64]. In this appendix we review the main results (especially from Refs. [10, 53, 56]) which are useful for the comparison with numerical results. We mention that some universal results are also known in higher dimensions both from field theory [65] and holography [63, 66, 67].

From global conformal invariance, we know that $\mathrm{Tr}\rho_A^n$ for two disjoint intervals admits the general scaling form (choosing, without loss of generality, the endpoints of the intervals in the order $u_1 < v_1 < u_2 < v_2$):

$$\mathrm{Tr}\rho_A^n = c_n^2 \left(\frac{(u_2-u_1)(v_2-v_1)}{(v_1-u_1)(v_2-u_2)(v_2-u_1)(u_2-v_1)} \right)^{2\Delta_n} \mathcal{F}_n(x), \tag{73}$$

where $\Delta_n = c(n-1/n)/12$, being c the central charge. The variable x is the four-point ratio

$$x = \frac{(u_1-v_1)(u_2-v_2)}{(u_1-u_2)(v_1-v_2)}. \tag{74}$$

Given the order of the points we have $0 \leq x \leq 1$. The prefactor c_n is non-universal, but can be exactly fixed from the exact calculation of the entanglement entropy of one interval.

The difficult task of CFT is to have an exact representation for the universal function $\mathcal{F}_n(x)$ normalised so that $\mathcal{F}_n(0)=1$. This universal function has been analytically derived for the compactified boson (with central change $c=1$) [52, 53] and for the Ising CFT (with $c=1/2$) [56, 57], as well as for other conformal theories which however are not of interest for this paper. Concerning the compactified boson, we are only interested in the value of the compactfication ratio corresponding to the scaling limit of the XX spin chain which is the so called Dirac point. For the Ising CFT and at the Dirac point (which describe respectively the scaling limit of the critical Ising chain and the critical XX model), the function $\mathcal{F}_n(x)$ reads [56]

$$\mathcal{F}_n^{\mathrm{Ising}}(x) = \frac{\sum_{\boldsymbol{e}} |\Theta[\boldsymbol{e}](\tau(x))|}{2^{n-1}\,|\Theta(\tau(x))|}, \qquad \mathcal{F}_n^{\mathrm{Dirac}}(x) = \frac{\sum_{\boldsymbol{e}} |\Theta[\boldsymbol{e}](\tau(x))|^2}{2^{n-1}\,|\Theta(\tau(x))|^2}, \tag{75}$$

where $\Theta[\boldsymbol{e}](\Omega)$ is the Riemann theta function, which is defined as follows [68]

$$\Theta[\boldsymbol{e}](\Omega) \equiv \sum_{\boldsymbol{m}\,\in\,\mathbb{Z}^{n-1}} e^{\,\mathrm{i}\pi(\boldsymbol{m}+\boldsymbol{\varepsilon})^{\mathrm{t}}\cdot\Omega\cdot(\boldsymbol{m}+\boldsymbol{\varepsilon})+2\pi\mathrm{i}\,(\boldsymbol{m}+\boldsymbol{\varepsilon})^{\mathrm{t}}\cdot\boldsymbol{\delta}}, \qquad [\boldsymbol{e}] \equiv \begin{bmatrix} \boldsymbol{\varepsilon} \\ \boldsymbol{\delta} \end{bmatrix} \equiv \begin{bmatrix} \varepsilon_1,\dots,\varepsilon_{n-1} \\ \delta_1,\dots,\delta_{n-1} \end{bmatrix}, \tag{76}$$

being Ω a $(n-1)\times(n-1)$ symmetric complex matrix with positive imaginary part and $\boldsymbol{e}$ is the characteristic of the Riemann theta function, which is defined by a pair of $n-1$

dimensional vectors made by $\varepsilon_i, \delta_i \in \{0, 1/2\}$. In Eq. (76) we have to sum over all the characteristics $\boldsymbol{e}$. The elements of the matrix $\tau(x)$ in Eq. (75) read [53]

$$\tau(x)_{rs} = \mathrm{i}\,\frac{2}{n}\sum_{k=1}^{n-1}\sin(\pi k/n)\,\frac{{}_2F_1(k/n, 1-k/n; 1; 1-x)}{{}_2F_1(k/n, 1-k/n; 1; x)}\,\cos\left[2\pi\frac{k}{n}(r-s)\right], \tag{77}$$

where $x \in (0,1)$ and ${}_2F_1$ is the hypergeometric function.

Also the moments of the partial transpose correspond to a four-point function of twist fields in which two of them have been interchanged [9]. Consequently also these moments admit the universal scaling form

$$\mathrm{Tr}(\rho_A^{T_2})^n \;=\; c_n^2 \left(\frac{(u_2-u_1)(v_2-v_1)}{(v_1-u_1)(v_2-u_2)(v_2-u_1)(u_2-v_1)}\right)^{2\Delta_n} \mathcal{G}_n(x), \tag{78}$$

with c_n the same non-universal constant appearing in Eq. (73) and $\mathcal{G}_n(x)$ a new universal scaling function. Exploiting the fact that the above moments correspond to the exchange of two twist fields, it has been shown that $\mathcal{G}_n(x)$ and $\mathcal{F}_n(x)$ are related as [9, 10]

$$\mathcal{G}_n(x) = (1-x)^{4\Delta_n}\mathcal{F}_n\left(\frac{x}{x-1}\right), \tag{79}$$

but some care is needed to take the analytic continuation of the function $\mathcal{F}_n(y)$ to negative argument y (see for details [10]). This result is equivalent to say that $\mathrm{Tr}(\rho_A^{T_2})^n$ is given by Eq. (75) in which the period matrix $\tau(x)$ is replaced by

$$\tau(x) \to \tilde{\tau}(x) = \tau\left(\frac{x}{x-1}\right). \tag{80}$$

Thus, the CFT prediction for ratio in Eq. (11) is

$$R_n^{\mathrm{CFT}}(x) = (1-x)^{4\Delta_n}\,\frac{\mathcal{F}_n(x/(x-1))}{\mathcal{F}_n(x)}, \tag{81}$$

in which the universal constants c_n as well as the dimensional part of the traces canceled out leaving a universal scale invariant quantity. Thus, in order to study this quantity we do not need an a priori knowledge of the constants c_n which anyhow are known both for the XX [32] and the Ising [33, 69] spin chains. It is worth recalling that the analytic continuation to non-integer n of the ratios (81) for two intervals are not yet known even for the simpler cases and consequently also the negativity is eluding an analytic description.

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