PhD Thesis:

Entanglement & Correlations in exactly solvable models

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Introduction

The phenomenon of entanglement is probably the most fundamental characteristic distinguishing the quantum from the classical world. It was one of the first aspects of quantum physics to be studied and discussed, and after more than 75 years from the publication of the classical papers by Einstein, Podolsky and Rosen [1] and by Schrödinger [2], the interest in the properties of entanglement is still growing. The quantum nature of entanglement makes difficult any intuitive description, and it is better to consider directly what it implies. Entanglement means that the measurement of an observable of a subsystem may affect drastically and instantaneously the possible outcome of a measurement on another part of the system, no matter how far apart it is spatially. The weird and fascinating aspect is that the first measurement affects the second one with infinite speed. After about 30 years from the appearance of concept of entanglement Bell published one of its most famous works [3] in which he showed that the entanglement forbids an explanation of quantum randomness via hidden variables, unraveling the EPR paradox, once and for all. But only 15 years later, when the Hawking radiation has been put in relation with the entanglement entropy, it has been realized that entanglement could provide unexpected information. The interest in understanding the properties of entangled states has received an impressive boost with the advent of “quantum information”, in nineties. For quantum information the entanglement is a resource, indeed quantum (non-local) correlations are fundamental e.g. for quantum teleportation or for enhancing the efficiency of quantum protocols [4]. The progress made in quantum information for quantifying the entanglement has found important applications in the study of extended quantum systems. In this context the entanglement entropy becomes an indicator of quantum phase transitions, and its behavior at different subsystem sizes and geometries uncovers universal quantities characterizing the critical points. In comparison with quantum correlation functions, the entanglement entropy measures the fundamental properties of critical neighborhoods in a “cleaner” way, e.g. the simple (linear) dependence of entanglement entropy on the central charge in a conformal system [5].

The thesis fits into this last genre of research. The next sections are devoted to introduce some general concepts that help understand the motivations for these studies. Firstly we overview the meaning of quantum phase transitions, secondly we give a non-technical introduction to the quench dynamics.
Quantum phase transitions

The concept of phase transition was introduced to describe the abrupt changes, from one state of matter to another, that a system undergoes at particular temperatures and pressures; the typical example being the first-order phase transitions between solid, liquid and gaseous phases. In classical models, they are driven by thermal fluctuations. In particular, continuous phase transitions are characterized by infinite correlation length: more and more distant points become correlated in the neighborhood of the critical temperature.

Quantum phase transitions deal with systems at temperature zero. As a matter of fact, thermal fluctuations are then absent, however quantum systems have fluctuations due to the Heisenberg uncertainty principle, which can drive the system under a quantum phase transition. Now, neither the temperature nor the pressure drives the transition, but some physical parameter, like an external magnetic field, or a coupling constant. In general, the properties of the ground state, first of all its energy, vary smoothly as the Hamiltonian’s parameters are changed. But there can be points in the parameter space in which the change is not analytic: these are called critical points. The existence of a critical point indicates that the properties of the state modify drastically crossing that point. For example a critical point could separate a ferromagnetic phase from a paramagnetic one. In addition, the low-lying excitations themselves can have a completely different nature.

It is easy to see the existence of critical points. For example we consider a system with a finite number of degrees of freedom with Hamiltonian \( H = H_0 + gH_1 \), where \( H_0 \) has a non-degenerate ground state. We assume \([H_0, H_1] = 0\, ,\, H_1 \neq H_0\), and without loss of generality \( \langle 0|H_1|0 \rangle = 0 \). An excited state \( |\Psi^*\rangle \) of \( H_0 \) such that \( \zeta = \langle \Psi^*|H_1|\Psi^*\rangle \neq 0 \) does exist, since \( H_1 \neq 0 \). In the set of excited states with this property, we consider the state \( |\Psi^*\rangle \) for which \( \frac{\omega}{\zeta} \) is minimum, where \( \omega = \langle \Psi^*|H_0|\Psi^*\rangle - \langle 0|H_0|0 \rangle \). \( g = \frac{\omega}{\zeta} \) is a critical point, or better a level crossing, indeed the ground state of \( H \) changes abruptly from \( |0\rangle \) to \( |\Psi^*\rangle \) in crossing that point, and the first derivative of the energy is discontinuous.

Actually, levels-crossing are not the most interesting kind of quantum criticality; on the contrary with “quantum critical point” is usually understood something different. In fact, if \( H_1 \) does not commute with \( H_0 \) levels-crossing can be avoided. But increasing the system’s size the energy difference between the levels could become progressively smaller so that eventually, in the limit of infinite system, the energy exhibits some non-analytic behavior. In particular, in the so-called second-order quantum phase transitions the characteristic energy scale \( \Delta \) of the state, which can be usually identified with the energy of the first excitation above the ground state, vanishes at the critical point. Generally, in the neighborhood of the critical point \( g_c \), \( \Delta \) has a power-law behavior and the exponent \( z\nu \) turns out to be independent of the microscopic details of the system, i.e. it is universal

\[
\Delta \approx |g - g_c|^{z\nu}.
\]
In addition, the correlation length diverges with the critical exponent $\nu$

$$\xi \approx |g - g_c|^{-\nu}. \quad (2)$$

so that

$$\Delta \approx \xi^{-z}. \quad (3)$$

$z$ is called the dynamical critical exponent. In the neighborhood of a critical point a universal quantum field theory describes the critical properties of the state. For example we consider a translational invariant system defined on a chain with lattice spacing $a$. The continuum limit $a \to 0$ can be done by defining some fields and some coupling constants that take finite values as the critical point is approached. Eventually, the system can be analyzed in the Lagrangian formalism introducing the Euclidian variables corresponding to space and imaginary time $\tau \equiv i t$.

Being interested in the long distance physics, we can trace out some short distance degrees of freedom. This can be done, for example, by restricting the momenta in the range $[e^{-\ell} \Lambda, \Lambda]$, where $\Lambda$ is a momentum cut-off introduced by the lattice and $e^{-\ell}$ is a rescaling factor. Our theory is finally valid only at lengths scales larger than $e^{\ell} a$. In simple cases the Lagrangian form can be kept by rescaling lengths $x \to e^{\ell} x$, imaginary times $\tau \to e^{z\ell} \tau$ and fields $\Psi \to e^{x\ell} \Psi$, for some $x\Psi$. Notice the crucial role played by the critical exponent $z$. In the special case of $z = 1$, when the dispersion relation of the low-lying excitations is linear $\varepsilon(k) \approx k$, space and time transform in the same way and the theory, defined in the two-dimensional Euclidian space $(x, \tau)$, is expected to be scale invariant. Moreover, as long as the original lattice model has sufficient symmetries, the theory in the continuum limit is invariant under infinitesimal rotations.

In fact, the universality hypothesis states that the universal properties, close to the phase transition, do not depend on microscopic details, but only on global properties, such as symmetries and dimensionality. It turns out that invariance under translations, rotations and scale transformations is usually accompanied by invariance under conformal transformations. This is a generalization of the scale transformation discussed above, in which the rescaling factor $e^{\ell}$ depends smoothly on space and time $a \to e^{(x,\tau)} a$. In two (Euclidian) dimensions $(x, \tau)$, conformal invariance is particularly powerful: if we use complex coordinates $z = x + i \tau$ and $\bar{z} = x - i \tau$ any analytic functions $z \to f(z)$ defines a conformal transformation. And this symmetry can be exploited to constraint the form of correlation functions. For example the two-point correlation function of a scalar primary field reads as

$$\langle \phi(\vec{r}_1)\phi(\vec{r}_2) \rangle \sim |\vec{r}_1 - \vec{r}_2|^{-2x_{\phi}}, \quad (4)$$

where $x_{\phi}$ is the scaling dimension of $\phi$. A theory invariant under conformal transformations is called CFT (conformal field theory) [7].

Summarizing, when $z = 1$ the universal features of critical one-dimensional systems (e.g. spin chains) can be obtained by studying the underlying CFT. In the thesis we face up continuously to CFT predictions, indeed most of the results presented in this work [8][9][10][11][12][13].
have been firstly obtained in that framework \cite{14,15,16}. On the other hand many features resulting from CFT calculations are not only characteristic of conformal systems, being observed in more general situations. For these reasons calculation for realistic models whose low-energy excitations are described by CFT become fundamental both for checking the correctness of the CFT predictions and for a better understanding of their meaning.

In Ref. \cite{9} we obtained the first exact numerical results for the Rényi entropies of disjoint subsystems and we established the exact relation between the reduced density matrix in the fermionic representation \textit{(i.e.} tracing out some fermionic degrees of freedom) and that in the spin representation, which is the actual reduced density matrix.

In Ref. \cite{11} we computed analytically the leading and sub-leading corrections to the scaling, up to $O(\ell^{-1})$, of the Rényi entropies in the XX chain with open boundary conditions. We also conjectured, and checked against numerics, a generalized Fisher-Hartwig for Toeplitz+Hankel matrices with the particular symbol characterizing the correlation matrix of the model.

In Ref. \cite{10} we investigated excited states of two integrable models. In particular we interpreted some excited states as ground states of conformal systems. We also studied the finite size scaling of the entanglement entropy in some excited states that behave in a very different way from the ground state of any Hamiltonian with short-range interaction.

In Ref. \cite{8} we studied the entanglement spectrum at “random singlet” 1D quantum critical points. The entanglement spectrum contains more information than the conventional entanglement entropy and Rényi entropies, and this is true in particular in the random singlet phase, where Rényi entropies do not provide further information other than the entanglement entropy.

Out-of-equilibrium quantum systems

The issue of equilibration of quantum systems has been firstly posed in a seminal paper by von Neumann in 1929 \cite{17}, but for long time it remained only an academic problem. Indeed, in solid state physics there are many difficulties in designing experiments in which the system’s parameters can be tuned. Moreover the genuine quantum features of systems could not be preserved for large enough times, because of dissipation and decoherence. Consequently, the research on quantum non-equilibrium problems blew over. Only in the last decade, the many-body physics of ultracold atomic gases overcome these problems: these are highly tunable systems, weakly coupled to the environment, so that quantum coherence is preserved for large times. In fact, a unique feature of many-body physics of cold atoms is the possibility to “simulate” quantum systems in which both the interactions and external potentials can be modified dynamically. In addition, the experimental realization of low-dimensional structures has unveiled the role that dimensionality and conservation laws play in quantum non-equilibrium dynamics. These aspects were addressed recently in a fascinating experiment on the time evolution of non-equilibrium Bose gases in one dimension, interpreted as the quantum equivalent of Newton’s cradle \cite{18}. 

One of the most important open problems is the characterization of a system that evolves from a non-equilibrium state prepared by suddenly tuning an external parameter. This is commonly called *quantum quench* and it is the simplest example of out-of-equilibrium dynamics. The time-dependence of the various local observables could be theoretically calculated from first principles, but in general this is a too hard task that cannot be solved even by the most powerful computers (incidentally, this is also the reason why quantum computers can be extremely more effective than classical ones). Insights can be obtained exploiting the most advanced mathematical techniques for low-dimensional quantum systems to draw very general conclusions about the quantum quenches. For example, if for very large times local observables become stationary (even though the entire system will never attain equilibrium), one could describe the system by an effective stationary state that can be obtained without solving the too complicated non-equilibrium dynamics. This is an intriguing aspect of quantum quenches that led to a vigorous research for clarifying the role played by fundamental features of the system, first of all integrability, that is to say the existence of an infinite number of conservation laws. The common belief is that in non-integrable systems (i.e. with a finite number of conservation laws) the stationary state can be described by a single parameter, that is an effective temperature encoding the loss of information about non local observables. Eventually the state at late times is to all intents and purposes equivalent to a thermal one with that temperature. This interesting picture opens the way for a quantum interpretation of thermalization as a local effective description in closed systems. When there are many (infinite) conserved quantities, as in integrable systems the effective temperature is not sufficient to describe the system’s features at late times. It is widely believed that the behavior of local observables could be explained by generalizations of the celebrated Gibbs ensemble [19].

In Ref. [12] we obtained the first exact (analytic) results for the entanglement entropies of large blocks in the XY model after a quench.

In Ref. [13] we determined analytically the large-distance behavior of the equal-time correlation functions after a quench for the paradigm of systems undergoing quantum phase transitions: the Ising model.
The thesis provides a survey of many important aspects of entanglement and quench dynamics in spin chains. The first part is intended as an overview of the subject; while the remainder is a presentation of our original contributions. It collects some of the results obtained in five papers, published during the PhD [8 9 10 11 13], and a preceding one [12]. However some material, in particular in the third chapter, is still unpublished.

In the first chapter we review the main properties of Rényi entropies, and in particular of the entanglement entropy. We discuss the meaning of strong subadditivity with respect to the subsystem’s geometry, that is to say, in 1D, the number of connected parts. Finally, we review the entanglement properties in the ground state of spin chains, pointing up the importance of analyzing the entanglement in critical systems.

In the second chapter, after a brief introduction to the so-called exactly solvable models and to the concept of integrability in quantum physics (especially in one dimension), we present the XY model. Some special features make the XY model the natural testing ground for analyzing the aspects of entanglement and of the out-of-equilibrium dynamics. Therefore, we collect in a single chapter many of the technical details that are fundamental in understanding the results obtained in different contexts.

The next chapters are almost independent: in each one a different aspect of entanglement is taken into account and the relative conclusions are drawn.

In the third chapter we present the results of Ref. [9]. We analyze the Rényi entropies of disjoint blocks, in particular in conformal systems. We describe an exact numerical method (the only available one, up to now) for determining the first integral Rényi entropies of disjoint subsystems in the thermodynamic limit and for large block’s lengths and distances. We come back to strong subadditivity in order to get bounds [20] for the universal function $F_{V,N}$, which is unknown for any model. We also provide an example of a system in which the universal functions display unusual behaviors [20].

In the fourth chapter we consider the question of corrections to the scaling. The importance of such studies relies on the fact that the exponents of the corrections in conformal systems turn out to be universal, being related to the scaling dimension of relevant operators of the theory. In addition, the knowledge of the form of the corrections can be useful in numerical studies in order to isolate the leading behavior. In particular, we report the results of Ref. [11], in which we have obtained the corrections to the scaling of Rényi entropies, in the open XX chain, up to $O(\ell^{-1})$.

In the fifth chapter we focus on the entanglement entropy of excited states. In fact, the entanglement in the ground state of Hamiltonians with short-range interactions has peculiar features distinguishing the ground state from a general pure state. Actually, even the excited states can not be considered completely general, and the behavior of the entanglement entropy of subsystems provides a classification of them. In Ref. [10] we have considered the excited states of XY Hamiltonians and we found two main classes, one in which the entanglement
entropies are extensive, and the other consisting of states that can be viewed as ground states of Hamiltonians with local interactions.

In the sixth chapter we investigate a different kind of criticality: that arising when quenched disorder is introduced in quantum systems. The averaged entanglement entropy is again a probe of criticality, displaying a universal behavior. Further information can be obtained by considering the entanglement spectrum. We present the results of Ref. [8], where we have studied the entanglement in random XX chains, obtaining information on some universal quantities that can not be inferred from the disorder average of the entanglement entropy (and of the Rényi entropies).

In the seventh chapter we introduce the simplest example of out-of-equilibrium dynamics: the quantum quench. We describe the common explanation of the phenomenon, focusing in particular on the behavior of the system late times after the quench. Reporting the results of Refs. [12] and [13], we check the correctness of the GGE (generalized Gibbs ensemble) hypothesis. We consider the time evolution of the entanglement entropy in the XY model and of the one- and two-point correlation functions in the Ising chain.
1. Entanglement Entropies: an Overview

In quantum mechanics, systems are described by states living in an appropriate Hilbert space. A useful concept is that of density matrix, usually denoted by \( \rho \): a positive semidefinite Hermitian operator with trace equal to 1. In particular, the density matrix \( \rho \) of a pure state \( |\Psi\rangle \) is a projector \( \rho^2 = \rho = |\Psi\rangle \langle \Psi| \). The properties of the state can be deduced from the expectation value of observables \( \hat{O} \)

\[
\langle \hat{O} \rangle \equiv \text{Tr} \rho \hat{O}, \tag{1.1}
\]

and if one would be able to perform sufficiently many measurements then the density matrix could be determined completely. The full knowledge of the density matrix is, however, an extremely hard task also in the most simple systems, and it is quite disputable whether such a business is worth for the understanding of the physical properties of the state. Indeed, for evident reasons, the operators \( \hat{O} \) associated to physical observables are local, that is to say they act non-trivially only on a limited spatial region. This means that we can trace out the faraway degrees of freedom and, eventually, the true quantities characterizing the state become the so-called reduced density matrices (RDM) of the subsystems.

The analysis of a few of observables, which could be two-point correlation functions and, in particular, the order parameter in quantum phase transitions, is usually sufficient to get the most important information about the state. However, many quantum features can be deduced by studying quantities that are not observables: \textit{e.g.} the von Neumann entropy and the Rényi entropies (from now on we’ll use the term “entanglement entropies” to indicate them both). They are functionals of the (reduced) density matrix with some fundamental properties, first of all the independence from the representation. They have been introduced to measure entanglement of a subsystem with the rest, but they have soon become an important means to uncover the fundamental features of the system.

We suppose that the Hilbert space can be written as a tensor product \( \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \). Let \( |\psi\rangle \) be a pure state in \( \mathcal{H} \). One of the most useful mathematical tools in understanding how to
1. ENTANGLEMENT ENTROPIES: AN OVERVIEW

quantify entanglement is the Schmidt decomposition, i.e.

$$|\psi\rangle = \sum_j \sqrt{p_j} |\psi_j\rangle_A \otimes |\psi_j\rangle_B ,$$

(1.2)

where $|\psi_j\rangle_{A(B)}$ are orthonormal vectors in $\mathcal{H}_{A(B)}$. The vector phases can be chosen in such a way to make $p_j$ real and positive. The square of the Schmidt coefficients \{p_j\} are the non-zero eigenvalues of A’s and B’s reduced density matrices

$$\rho_{A(B)} = \text{Tr}_{A(B)} \rho .$$

(1.3)

The entanglement between $A$ and $B$, as long as the system is in the pure state $|\psi\rangle$, is characterized entirely by the set \{p_j\}.

In fact, the eigenvalues of the reduced density matrices are strongly influenced by the quantum features of the system. And the entanglement entropies measure quantum correlations without any reference to the system, in contrast to the worldly-wise choice of observables that has to be done in order to achieve analogous goals\(^1\).

This is only partially true when the state is not pure: the entanglement entropies of subsystems in a mixed state do not measure the entanglement, since classical correlations have an impact on the result. This can be understood intuitively observing that the density matrix at inverse temperature $\beta$ describes a mixed state

$$\rho(\beta) = \frac{e^{-\beta H}}{\text{Tr} e^{-\beta H}} ,$$

(1.4)

where $H$ is the Hamiltonian, and in the limit of large temperatures it coincides with the classical concept of statistical ensemble.

For these reasons the entanglement entropies are powerful tools mainly in characterizing (pure) states at temperature zero, and in particular quantum phase transitions. For example, it is noteworthy that the entanglement entropies of large subsystems in 1+1 conformal systems are proportional to the central charge of the underlying conformal field theory (CFT) and independent of non-universal details\([5\,21]\). Thus the entanglement entropies provide one of the clean ways of detecting, for example, the central charge.

In addition, sometimes just the structure of the density matrix is sufficient to compute the entanglement entropies, without knowing the full spectrum and, even worse, every matrix element. This means that the calculation of the entanglement entropies in such systems (e.g. the XY model\([9\,22\,23]\)) can be done efficiently.

\(^1\)In a quantum field theory the entanglement entropies are related to the correlation functions of particular fields, twist fields, lying on the boundaries of the subsystem (cf. Sec. 1.2.1). In particular, in conformal systems the entanglement entropies can be evaluated by considering the correlation functions of the twist fields with the stress tensor, which is always defined in any theory.
**Entanglement entropies.** The *von Neumann entropy*, commonly called *entanglement entropy*, is defined as

\[ S_{v.N.} \equiv - \text{Tr} \rho \log \rho, \quad (1.5) \]

where \( \rho \) is a general density matrix, while the *Rényi entropies* constitute the family of entropies, depending on the real parameter \( \alpha \),

\[ S_{\alpha} \equiv \log \text{Tr} \rho^\alpha / (1 - \alpha). \quad (1.6) \]

Rényi entropies turn out to be continuous functions of the parameter \( \alpha \) for \( \alpha \geq 1 \), so the entanglement entropy can be obtained from the Rényi entropies as the right limit of \( S_{\alpha} \) as \( \alpha \) approaches 1

\[ S_{v.N.} = \lim_{\alpha \to 1^+} S_{\alpha}. \quad (1.7) \]

They are differentiable in the region \( \alpha > 1 \), and hence the entanglement entropy can be also expressed in terms of the first derivative with respect to \( \alpha \), in the limit as \( \alpha \) approaches 1

\[ S_{v.N.} = - \lim_{\alpha \to 1^+} \frac{\partial}{\partial \alpha} S_{\alpha}. \quad (1.8) \]

There are many properties common to both Rényi entropies and the entanglement entropy, here a brief about the most important ones [24]:

- **positivity:** they are greater or equal to 0, and they vanish iff (if, and only if) the state is pure

\[ S_{\alpha} \geq 0 \quad \rho^2 = \rho \Leftrightarrow S_{\alpha} = 0; \quad (1.9) \]

- **invariance:** they depend on the (strictly) positive part of the density matrix. This means, in particular, that they are invariant under unitary transformations and under the expansion of the space \( H \to H \oplus H' \) in which \( \rho \to \rho \oplus 0 \)

\[ S_{\alpha}[U \rho U^\dagger] = S_{\alpha}[\rho] \quad UU^\dagger = I, \]

\[ S_{\alpha}[\rho \oplus 0] = S_{\alpha}[\rho]. \quad (1.10) \]

Because of this, the entanglement entropies of a subsystem \( A \), of a system prepared in a pure state, are equal to the entanglement entropies of the rest \( \bar{A} \) of the system

\[ S_{\alpha}[\rho_A] = S_{\alpha}[\rho_{\bar{A}}]; \quad (1.11) \]

- **insensitivity:** they are continuous functions of finitely many eigenvalues, provided that the rest of them are kept fixed. This property is crucial to infer some properties of the distribution of the RDM’s eigenvalues on the basis of the behavior of the entanglement entropies (*e.g.* in Ref. [25]).
1. ENTANGLEMENT ENTROPIES: AN OVERVIEW

There is, however, a property peculiar to the von Neumann entropy: strong subadditivity, with all other weaker resulting properties, like subadditivity.

Strong subadditivity puts in relation the entanglement entropy of three subsystems $A$, $B$, and $C$ with empty intersection:

$$S_{v.N.}[A \cup B \cup C] + S_{v.N.}[B] \leq S_{v.N.}[A \cup B] + S_{v.N.}[B \cup C].$$

(1.12)

Subadditivity is a direct consequence of strong subadditivity, and can be recovered by substituting $B$ with the empty space and using $S_{v.N.}[\emptyset] = 0$

$$S_{v.N.}[A \cup C] \leq S_{v.N.}[A] + S_{v.N.}[C];$$

(1.13)

subadditivity means that the entanglement entropy can be extensive at the most.

In the study of extended quantum systems, the entanglement entropies are a probe into the universal features of critical systems, as well as indicators of quantum phase transitions; therefore, distinguishing the properties, ascribed to the particular system under examination, from those that result from just the definition of the entropies is essential. This is the spirit of the two following sections: in the former we discuss the meaning of strong subadditivity with regard to the subsystem’s structure, in the latter we overview the behavior of the entanglement entropies in the ground state of one dimensional systems.

1.1 Strong subadditivity

In this section we show how strong subadditivity constrains the dependence of the entanglement entropy on the subsystem’s geometry. We focus on systems with one spatial dimension, but we also give some comments about the generalizations to higher dimensions.

In one dimension a set of lengths characterizes completely a subsystem: if the subsystem is connected then we need only the position $r$ and its extent $\ell$, otherwise we need the same information but for all its connected parts. The natural way to look at strong subadditivity is to order the relations by minimizing the number of lengths involved: the more the lengths characterizing the subsystem are, the less the entanglement entropy is constrained.

In fact the available analytical and numerical results for the entanglement entropies in 1D suggest that the general behavior of entropies depends on the number of intervals. Thus, a systematic study of the implications of strong subadditivity at fixed number of connected components could be useful e.g. for providing bounds to the universal quantities characterizing the critical system.

For the sake of simplicity we focus on systems prepared in the ground state of “quasi”-translational invariant Hamiltonians, where “quasi” means that the 1D system is, in general, a chain (lengths are proportional to the lattice spacing $a$, hence only translations multiple of $a$ make sense) and one or two boundaries could spoil the symmetry.
1.1 Strong subadditivity

Many of the results presented in the following sections are widely known (especially those about single intervals [30]), however the classification according to the number of connected components has not yet been investigated, basically because the study of the entanglement entropy of disjoint intervals in 1D has just started. In view of this gap, we intend to provide an exhaustive analysis of strong subadditivity which starts with these introductory sections and will continue in Chapter 3, in which the entanglement of two disjoint intervals is thorough.

1.1.1 Periodic boundary conditions

In a periodic chain the entanglement entropy depends on the positions of the subsystem’s connected parts only through their distances \( r_i - r_j \), where \( i \) and \( j \) run over the parts. In particular the entanglement entropy of a connected subsystem depends only on the subsystem’s length \( \ell \).

**Connected subsystems.** There is only a choice of subsystems for which strong subadditivity puts in relation connected regions, i.e. when \( A \) is adjacent to \( B \) and \( B \) to \( C \) (we depict this configuration as \( ABC \)): by substituting the lengths in Eq. (1.12) we get

\[
S(\ell_A + \ell_B + \ell_C) + S(\ell_B) \leq S(\ell_A + \ell_B) + S(\ell_B + \ell_C). \tag{1.14}
\]

The meaning of the inequality can be easily understood by recasting the expression as follows\(^1\)

\[
\left[ e^{\ell_C \frac{\pi}{\ell_A}} - 1 \right] \left[ e^{\ell_A \frac{\pi}{\ell_C}} - 1 \right] S(\ell) \leq 0; \tag{1.15}
\]

the variation of entanglement entropy resulting from decreasing the subsystem’s length is a decreasing function of the length. In particular, in the limit as both \( \ell_C \) and \( \ell_A \) approach 0, we get the concavity condition

\[
S''(\ell) \leq 0. \tag{1.16}
\]

We stress Eq. (1.16) is weaker than (1.15), indeed the latter inequality rules out the possibility of oscillations also if they have characteristic periods of the order of the lattice spacing \( a \).

In the limit \( \ell_B \to 0 \) and finite \( \ell_A \) and \( \ell_C \) we get subadditivity

\[
S(\ell_A + \ell_C) \leq S(\ell_A) + S(\ell_C), \tag{1.17}
\]

that is

\[
S(\ell) \leq \frac{\ell}{a} S(a). \tag{1.18}
\]

Notice that these results are completely independent of the physical details.

Here some comments about the generalization to higher dimensions. Subadditivity has almost the same meaning in any dimension

\[
S[R] \leq \frac{V_R}{V_{R_0}} S[R_0], \tag{1.19}
\]

\(^1\)Although the appearance of operators could be annoying, factorization is good, resolving the sum of entropies into elementary operations
where $R$ consists of $\frac{V_R}{V_{R_0}}$ elementary regions $R_0$ put together, and we indicated by $V_A$ the volume of the region $A$: the entanglement entropy is always bounded from above by the volume.

On the other hand strong subadditivity does not mean that the entanglement entropy is a concave function of any subsystem’s parameter. For example circles in two dimensions are characterized by the radius, but there is no way to write a relation from (1.12) that puts in relation the entanglement entropy of just circles. And in this simple case strong subadditivity does not imply directly the concavity with respect to the radius. However, because of strong subadditivity, the entanglement entropy of rectangles is a concave function of the lengths of their sides.

**Disjoint subsystems.** In the previous paragraph we discussed the meaning of strong subadditivity for connected subsystems in a periodic chain. We found a very simple property, concavity, that discriminates the Rényi entropies from the entanglement entropy. Now we consider subsystems made of many (connected) blocks.

It is worth recalling that in the case of many intervals, the entanglement entropy measures only the entanglement of the disjoint intervals with the rest of the system. It is not a measure of the entanglement of one interval with respect another, which instead requires the introduction of more complicated quantities \(^{[31,32]}\): the disjoint subsystem is in a mixed state, hence the Schmidt decomposition cannot be done.

From a different point of view, the entanglement of disjoint intervals in a theory with local interactions can be seen as the entanglement of a connected subsystem in which additional non-local interactions between a few sites \(^1\) switch on (in particular, at some subsystem’s boundaries). The appearance of non-local terms suggests that the behavior of the entanglement entropies could depend on the very number of connected components.

The entanglement entropy of a disjoint subsystem in a periodic chain depends on $2N - 1$ lengths, where $N$ is the number of connected components. Strong subadditivity \(^{[1,12]}\), however, is a relation between the entanglement entropy of the subsystems $A \cup B \cup C$, $B$, $A \cup B$, and $B \cup C$, hence the inequality could involve up to $6N - 1$ lengths. Actually, the most general inequalities, for a given maximal number $n_{\text{max}}$ of connected components of the four subsystems, can be written in terms of a smaller number of lengths. This can be seen by considering the following expansion

$$
\Delta^{(B)}_{A,n} \equiv S\left[\left(\bigcup_{i=1}^{n} A_i\right) \cup B\right] - S[B] = \left\{S\left[\left(\bigcup_{i=1}^{n} A_i\right) \cup B\right] - S\left[\left(\bigcup_{i=1}^{n-1} A_i\right) \cup B\right]\right\} + \Delta^{(B)}_{A,n-1}, \quad (1.20)
$$

where $A_i$ are the connected regions of $A$. The term in bracket on the r.h.s. is the difference between the entanglement entropy of two regions that differ for a single connected region ($A_n$),

\(^{1}\)The new system can be obtained by permuting some regions of the chain.
and the recurrence equation is solved by the sum of $n$ terms of this kind. Strong subadditivity can be written as $\Delta^{(B_{m,n})}_{A_{m,n}} - \Delta^{(B)}_{A_{m,n}} \leq 0$, i.e.

$$\sum_{n=1}^{n_A} \sum_{m=1}^{n_C} \left\{ S\left( \bigcup_{i=1}^{n} A_i \right) \cup B \cup \left( \bigcup_{i=1}^{m} C_i \right) \right\} - S\left( \bigcup_{i=1}^{n} A_i \right) \cup B \cup \left( \bigcup_{i=1}^{m} C_i \right) \leq 0.$$  \hbox{(1.21)}

Defining the regions $\bar{B}_{n,m} = (\bigcup_{i=1}^{n} A_i) \cup B \cup (\bigcup_{i=1}^{m} C_i)$, strong subadditivity for the original disjoint subsystems $A$, $B$, and $C$ can be traced back to strong subadditivity for the regions $A_n$, $C_m$, and $B_{nm}$ with $\leq n_A$ and $m \leq n_C$

$$S[A_n \cup \bar{B}_{nm} \cup C_m] + S[\bar{B}_{nm}] \leq S[A_n \cup \bar{B}_{nm}] + S[\bar{B}_{nm} \cup C_m]. \hbox{(1.22)}$$

In other words the inequalities (1.22) give any information enclosed in (1.12) when the subsystems $A \cup B \cup C$, $A \cup B$, and $B \cup C$ consist of no more than $n_{\text{max}}$ intervals. For example, the results obtained in the previous paragraph correspond to set $n_{\text{max}}$ equal to 1. For $n_{\text{max}} = 2$ we find relations between subsystems consisting of two or less connected parts, and so on.

The expansion (1.21) can be useful because, in contrast to the original inequality in which $A$ and $C$ can have many connected components, now $A_n$ and $C_m$ are intervals. However, in Eq. (1.21), terms with a larger number of disjoint parts could appear because of $\bar{B}_{nm}$ (eventually, they must simplify). The question is whether or not an ordering for the connected regions of $A$ and $C$ exists such that all the regions in Eq. (1.22) consist of no more than $n_{\text{max}}$ connected components, that is to say, all subsystems of the form $(\bigcup_{i=1}^{n} A_i) \cup B \cup (\bigcup_{i=1}^{m} C_i)$ are made of $n_{\text{max}}$ blocks or less.

In fact such an ordering exists, as we are going to prove by induction. For $n \in \{0, n_A\}$ and $m \in \{0, n_C\}$ this is true by hypothesis: \{\{n, m\} = \{0, 0\} corresponds to the subsystem $B$, \{\{n, m\} = \{0, n_C\} to $B \cup C$, \{\{n, m\} = \{n_A, 0\} to $A \cup B$, and \{\{n, m\} = \{n_A, n_C\} to $A \cup B \cup C$. We now prove by \textit{reductio ad absurdum} that, assuming it is true for $n$ (and $m$, considering the region $C$), it must be true also for $n - 1$ (as well as for $m - 1$). Indeed, if we can not remove a block $A_j \leq n$ without increasing the number of connected components then every connected region of $\bigcup_{i}^{n} A_i$ must be surrounded by other blocks (if empty spaces are adjacent to some $A_j$, then the number of connected regions after removing $A_j$ does not increase). If this were true, removing the entire region $\bigcup_{i}^{n} A_i$ will lead to a larger number of disjoint parts, but this is absurd because, by hypothesis, for $n = 0$ the number of connected components is not greater than $n_{\text{max}}$. The same argument holds for $m$; thus the theorem is proved, and we get the following result:

Every inequality, obtained from strong subadditivity (1.12) by considering subsystems $A \cup B \cup C$, $A \cup B$, and $B \cup C$ with $n_{\text{max}}$ connected components at the most, can be deduced from the configurations in which $B$ is made of $n_{\text{max}}$ connected parts, and $A$ and $C$ are connected and adjacent to $B$. Indeed, these are the configurations maximizing the connected components (they are all equal to $n_{\text{max}}$).
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In particular, if \( n_{\text{max}} = 2 \), the subsystem configurations that can be expected to give independent inequalities are

\[
BA, BC \quad \text{and} \quad B, ABC,
\]

where the symbol \( - \) means that the regions to the left and to the right are detached, and we exploited the periodicity and Eq. 1.11 to discard configurations like \( AB, BC \). Finally, substituting the corresponding lengths into Eq. 1.12 we get

\[
S(\ell_B + \ell_A; r; \ell'_B + \ell_C) + S(\ell_B; \ell_A + r; \ell'_B) \leq S(\ell_B + \ell_A; r; \ell'_B + \ell_C) + S(\ell_B; \ell_A + r; \ell'_B + \ell_C)
\]

where the symbol \( S(\ell_B; \ell_A; r; \ell'_B + \ell_C) \) is the entanglement entropy of two blocks, \( \ell_B \) and \( \ell'_B \) in length, at the distance \( r \). The inequalities can be recast as follows

\[
\left( e^{\ell_C \frac{\partial}{\partial u_1}} - 1 \right) \left( e^{\ell_A \frac{\partial}{\partial u_2}} - e^{\ell_A \frac{\partial}{\partial v_1}} \right) S(\ell_B; \ell_A; r; \ell'_B) \leq 0
\]

\[
\left( e^{\ell_C \frac{\partial}{\partial v_2}} - 1 \right) \left( e^{\ell_A \frac{\partial}{\partial u_1}} - e^{\ell_A \frac{\partial}{\partial v_1}} \right) S(\ell_B; \ell_A; r; \ell'_B) \leq 0
\]

(1.24)

the variation of entanglement entropy, resulting from moving the inner boundary of one block in order to decrease the distance, is a decreasing function of the length of each block.

In the limit in which \( \ell_B \) and \( \ell'_B \) approach 0 we get subadditivity

\[
S(\ell_A; r; \ell_C) \leq S(\ell_A) + S(\ell_C),
\]

which means that the entanglement entropy of two disjoint blocks is bounded from above by the sum of the entanglement entropies of each block.

Indicating by \( u_i, v_i \) \( (v_i > u_i) \) the boundaries of the \( i^{th} \) block, strong subadditivity can be rewritten as follows:

\[
\frac{\partial^2}{\partial u_i \partial u_j} S \leq 0 \quad \frac{\partial^2}{\partial u_i \partial v_j} S \geq 0 \quad \frac{\partial^2}{\partial v_i \partial v_j} S \leq 0.
\]

(1.27)

This result can be easily generalized to an arbitrary number of disjoint blocks, indeed \( A \) and \( C \) continue to be adjacent to \( B \).

Finally, we can conclude that, irrespective of the number of connected components (but also of boundary conditions) strong subadditivity is completely equivalent to the following inequalities (where derivatives must be interpreted as finite displacements):

\[
\frac{\partial^2}{\partial u_i \partial u_j} S \leq 0 \quad \frac{\partial^2}{\partial u_i \partial v_j} S \geq 0 \quad \frac{\partial^2}{\partial v_i \partial v_j} S \leq 0 \quad i, j \leq n_{\text{max}},
\]

(1.28)

the variation of entanglement entropy, resulting from moving a boundary in the outer direction, i.e. increasing the block’s length, decreases as another boundary is moved in the outer direction.
1.1 Strong subadditivity

1.1.2 Open boundary conditions

In this section we consider chains with open boundary conditions, which could be semi-infinite, with one boundary, or finite, with two boundaries. The typical system is a periodic chain in which the interaction between two sites (we are assuming nearest-neighbor interaction) is switched off.

Actually, the inequalities (1.28) are expressed in terms of subsystem’s boundaries (not in terms of distances), hence they are still valid (we have not used periodicity).

In contrast to the periodic case, the entanglement entropy in a chain with open boundary conditions depends also on the distance of the subsystem from the boundary. The dependence on the position carries with it the impossibility to write an inequality for connected blocks at a given distance, for example blocks starting from the boundary. Indeed, we should append two blocks A and C to the connected block B, leaving it connected, but only one block’s boundary is available. For connected blocks, strong subadditivity implies (we are considering the configuration $oABC$, where $o$ indicates the boundary)

$$S(\ell_A + \ell_B + \ell_C | r_0 - \ell_A) - S(\ell_A + \ell_B | r_0 - \ell_A) \leq S(\ell_B + \ell_C | r_0) - S(\ell_B | r_0),$$  \hspace{1cm} (1.29)

where $S(\ell | r)$ is the entanglement entropy of a block $\ell$ in length, at the distance $r$. In other words, the variation of entanglement entropy, resulting from decreasing the subsystem’s length, increases as the first subsystem’s boundary is moved away from the boundary. In particular, strong subadditivity does not imply any more that the entanglement entropy is a concave function of the block’s length. Putting $\ell_B$ to 0 we get subadditivity

$$S(\ell_A + \ell_C | r_0 - \ell_A) - S(\ell_A | r_0 - \ell_A) \leq S(\ell_C | r_0),$$  \hspace{1cm} (1.30)

but also in this case, because of the dependence on the distance, the inequality is inappropriate to constrain the behavior of the entanglement entropy of a block joined to the boundary.

In conclusion, oscillations in the entanglement entropy of a connected subsystem are not forbidden when open boundary conditions are imposed. Moreover, as for disjoint blocks in a chain with periodic boundary conditions, more lengths come into play and the interpretation of strong subadditivity becomes more involved.

In the following chapters we will see that oscillations are indeed present, e.g. in the XX chain with open boundary conditions. In addition, we will see that the absence of oscillations in the same model but with periodic boundary conditions is peculiar to the entanglement entropy: the corrections to the scaling for the Rényi entropies oscillate. Regarding disjoint blocks, the meaning of the inequalities (1.27) will be reinterpreted on the basis of the CFT predictions in conformal systems.

In the following section we review the basic features of the entanglement entropies in the ground state of quantum spin chains. The behavior of the entanglement entropies in excited states will be examined in a separate chapter.
1. ENTANGLEMENT ENTROPIES: AN OVERVIEW

1.2 Entanglement entropies in the ground state of quantum spin chains

The properties of the entanglement entropy introduced in the previous sections indicate that the entanglement entropy of a subsystem $A$ in a chain can be extensive (proportional to its length $\ell_A$) and, if $A$ is connected, must be a concave function of $\ell_A$. In fact it is straightforward to construct reduced density matrices with extensive entanglement entropies, e.g. the maximal entangled state corresponds to an RDM proportional to the identity

$$\rho = \frac{1}{|\mathcal{H}_A|} \quad \Leftrightarrow \quad S_\alpha = \log |\mathcal{H}_A|, \quad (1.31)$$

where $|\mathcal{H}_A|$ is the size of the Hilbert space associated to the region $A$, (e.g., in a spin-$\frac{1}{2}$ chain $|\mathcal{H}_A|$ is equal to $2^{\ell_A}$). Moreover, it is also simple to find Hamiltonians whose ground state has extensive entropy, and in Chapter 5 on the entanglement in excited states, we’ll construct a family of them explicitly. However such Hamiltonians have non-local interactions.

Indeed, generally, as long as we are in the ground state and the interaction is local, the entanglement entropy (but also the Renyi entropies) satisfies the area law [33]: the entanglement entropy of a subsystem scales as the area of the contact surface with the rest of the system. In fact it is expected that the entanglement will be created between the degrees of freedom in the neighborhood of the subsystem’s surface, and hence any measure of entanglement must scale as the area. This is indeed true for non critical systems, in which the dispersion relation is gapped and the correlation length finite.

In 1D this means that the entanglement entropy becomes soon independent of the subsystem’s length, wherever that length is larger than the correlation length $\xi$. In particular, for sufficiently large correlation lengths, the following scaling is observed [5]

$$S_{v.N.}[A] \sim \mathcal{A} \frac{c}{6} \log \frac{\xi}{a} \quad \ell_{A_j}, \ell_{\bar{A}_j} \gg \xi \gg a \quad (1.32)$$

where $\ell_{A_j}$ ($\ell_{\bar{A}_j}$) is the length of the $j^{th}$ connected region of $A$ (the rest of the system $\bar{A}$), and $\mathcal{A}$ is the number of subsystem’s boundaries. $c$ is a constant, which turns out to be universal if the system is close to a phase transition, being the central charge of a conformal field theory.

On the other hand if the typical subsystem’s length is much less than the correlation length (but much larger than the ultraviolet cut-off $a$) the system can be assumed to all intents and purposes critical: the energy dispersion of the low-lying excitations is effectively gapless and, under some hypotheses, it can be described by a CFT. In section 1.2.1 we show that the entanglement entropies of an interval in a conformal system scale as

$$S_\alpha[A] \sim \frac{1 + \alpha}{\alpha} \frac{c}{6} \log \frac{\ell_A}{a}. \quad (1.33)$$

The result, however, is more general. Indeed there are physical systems that are critical (with divergent correlation length, i.e. gapless dispersion relation), but because of the explicit breaking of some symmetries, like translational or rotational invariance, are not conformal. In section
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1.2.2 we consider an example of systems, random quantum systems, in which translational invariance is broken by quenched disorder, but the disorder averaged entanglement entropies grow as the logarithm of the subsystem’s lengths. Translation invariance is also broken by taking aperiodic couplings, for instance; and conformal invariance is broken by theories with gapless parabolic dispersion relations, in which, instead, translational invariance can be unbroken. In fact, in any critical system analyzed up to now the entanglement entropies of an interval grow as the logarithm of the subsystem’s length

\[ S_\alpha [A] \propto \log \frac{\ell_A}{a}, \]

where the proportionality constant is universal, in the sense that it is independent of the lattice spacing \( a \).

In conclusion, it is expected that the entanglement entropies of an interval in the ground states of quantum spin chains have the general behavior

\[ S_\alpha [A] \sim f(\alpha) \log \frac{\ell_A}{a} + c_\alpha', \]

where \( f(\alpha) \) is universal and non-zero only if the system is critical, while \( c_\alpha' \) can depend on non-universal details of the system. We stress that the Rényi entropies have the same dependence on \( \ell_A \) than the entanglement entropy. In particular they are concave functions of the subsystem’s length, as well as the entanglement entropy is (and must be, because of strong subadditivity). This is quite surprising in view of the fact that Rényi entropies are not even subadditive. We’ll see that concavity is indeed broken by the corrections to the scaling.

1.2.1 Conformal systems

In this section we overview the “geometric” interpretation of Rényi entropies in a quantum field theory and then we sketch out the fundamental role played by conformal symmetry in obtaining the asymptotic behavior of Rényi entropies, and in particular of the entanglement entropy. See Refs. [34, 35] for a detailed review on these subjects.

Path integral formulation. We indicate with \( \{ \hat{\phi}_x \} \) a complete set of local commuting observables, where \( x \) is a discrete variable labeling the lattice sites. We denote by \( \{ \phi_x \} \) and \( | \{ \phi_x \} \rangle \) their eigenvalues and eigenvectors, respectively. For example in a spin model the local operator \( \hat{\phi}_x \) turns out to be a component of the local spin. The representation of the density matrix

\[ \rho = \frac{e^{-\beta H}}{Z(\beta)}, \quad Z(\beta) = \text{Tr} e^{-\beta H}, \]

at inverse temperature \( \beta \), in the basis consisting of the states \( \otimes_x |\{ \phi_x \} \rangle = |\prod_x \{ \phi_x \} \rangle \), can be written as a path integral on the imaginary time interval \((0, \beta)\)

\[ \langle \{ \phi_x \} | \rho | \{ \phi'_x \} \rangle = \frac{1}{Z} \int [d\phi(y, \tau)] \prod_y \delta(\phi(y, 0) - \phi'_y) \prod_y \delta(\phi(y, \beta) - \phi_x) e^{-f_0^y \mathcal{L} d\tau}, \]

with \( \mathcal{L} \) the Euclidian Lagrangian. The constant \( Z \) is the partition function and ensures the normalization; it is obtained by taking the trace of the path integral

\[ Z = \int [d\phi(y, \tau)] \prod_y \delta(\phi(y, \beta) - \phi(y, 0)) e^{-f_0^y \mathcal{L} d\tau} \xrightarrow{a \to 0} \int [d\phi(x, \tau)] e^{-\int \mathcal{L}[\phi(x, \tau)]} \int [d\phi(x, \tau)] e^{-\int \mathcal{L}[\phi(x, \tau)]}. \]

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In the continuum limit $a \to 0$, the path integral is over fields $\phi(x)$ that lie in the Riemann surface $\mathcal{R}$ corresponding to the cylinder of circumference $\beta$, obtained by sewing together the edges along $\tau = 0$ and $\tau = \beta$. Here $\mathcal{L}[\phi]$ is the local Lagrangian density.

In fact the reduced density matrix of the subsystem $A$ is a partial trace of the density matrix, and can be obtained by setting $\{\phi_y^x\} = \{\phi_y^x\}$ for all $x \in \mathcal{R}_{n}[A]$

$$\langle\{\phi_y^x\}_{A} | \rho_{A} | \{\phi_y^x\}_{A'}\rangle = \int \frac{[d\phi(y,\tau)]}{Z} \prod_{y \notin A} \delta(\phi(y,\beta) - \phi(y,0)) \prod_{y \in A} \delta(\phi(yA,0) - \phi_x^A) e^{-\int_{0}^{\beta} \mathcal{L}d\tau},$$

(1.38)

where we highlighted the variables in $A$ with the subscript $A$. The path integral formulation is convenient to represent the trace of the $\rho_{A}$'s moments $\text{Tr} \rho_{A}^{n}$. Indeed the product of two density matrices $\rho_{A}^{(1)} \rho_{A}^{(2)}$ can be obtained by equating $\phi_{1}(y,\beta)$, of $\rho_{A}^{(1)}$, with $\phi_{2}(y,0)$, of $\rho_{A}^{(2)}$, wherever $y \in A$. The trace is nothing else but a further product between the last density matrix and the first one.

This means that, in the continuum limit, $Z^{n} \text{Tr} \rho_{A}^{n}$ is the path integral over fields $\phi(x,\tau)$ on an $n$-sheeted Riemann surface $\mathcal{R}_{n}[A]$, with branch points at $A$’s boundaries

$$Z_{n}[A] \equiv Z^{n} \text{Tr} \rho_{A}^{n} = \int_{\mathcal{R}_{n}[A]} [d\phi(x,\tau)] e^{-\int_{\mathcal{R}_{n}[A]} \mathcal{L}[\phi](x,\tau)}.$$  

(1.39)

By using Eq. (1.39) to define some fields in $\mathbb{C}$ that incorporate the structure of the Riemann surface (in a sense, by specifying their correlations functions as given by Eq. (1.39)), they would be non-local (this is somehow related to the non-local nature of the branch cut$^{1}$). However, many results on integrable quantum field theories rely on locality, hence locality is an important feature to recover. The problem is solved by enlarging the model in such a way that our fields are now defined in a model formed by $n$ independent copies of the original one.

Finally, the partition function (1.39) can be rewritten as the path integral on the complex plane

$$Z_{n}[A] = \int_{\mathcal{Z}_{n}[A]} [d\varphi_{1} \cdots d\varphi_{n}] \exp \left[ - \int_{\mathbb{C}} dxd\tau (\mathcal{L}[\varphi_{1}](x,\tau) + \cdots + \mathcal{L}[\varphi_{n}](x,\tau)) \right],$$

(1.40)

where $\int_{\mathcal{Z}_{n}[A]}$ means that the path integral is restricted by the conditions

$$\varphi_{j}(x,0^{+}) = \varphi_{j+1}(x,0^{-}), \quad x \in A, \quad j = 1, \ldots, n,$$

(1.41)

and $n + j \equiv j$. In writing Eq. (1.40) we have taken the limit $\beta \to \infty$. The fields defined implicitly in (1.40) are local. They are specific twist fields, denominated “branch-point twist fields”. Twist fields $\mathcal{T}_{\sigma}$ exist in any quantum field theory with a global internal symmetry $\sigma$.

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$^{1}$The correlation function between these fields and the energy density (obtained inserting the Lagrangian density into the path integral), is not defined in $\mathbb{C}$, since bringing the Lagrangian density around a branch point modifies the correlation function $^{36}$. 

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*i.e.* a symmetry that acts in the same way everywhere in space, preserving the positions of fields, \( \int dx d\tau \hat{L}[\sigma \varphi](x, \tau) = \int dx d\tau \hat{L}[\varphi](x, \tau) \). They are defined formally by their correlation functions

\[
\langle \mathcal{T}_\sigma(x, \tau) \cdots \rangle \propto \int_{\mathbb{R}^n} [d\varphi] \exp \left[ - \int_{\mathbb{R}^n} dx' d\tau' \mathcal{L}[(x', \tau')] \right] \cdots ,
\]

where the dots represent the insertions of other local fields. With notation analogous to that in Eq. (1.40), we indicated with \( \int_{\mathbb{R}^n} \) the restricted path integral with conditions

\[
\varphi(x', \tau^+) = \sigma \varphi(x', \tau^-) \quad x' \in [x, \infty)
\]

Actually, the twist fields defined by Eq. (1.42) are not the most general ones (for example we could insert a field \( \varphi \) in the path integral), but they have the lowest scaling dimension: they are primary, in the language of conformal field theory (see Ref. [36] and references therein for an insightful discussion on twist fields and locality).

In the specific model (1.40) the *branch-point twist fields* are associated to the symmetry under the cyclic permutations of the copies

\[
\mathcal{T}_n = \mathcal{T}_{\sigma}, \quad \sigma : i \mapsto i + 1 \mod n
\]

\[
\tilde{\mathcal{T}}_n = \mathcal{T}_{\sigma^{-1}}, \quad \sigma^{-1} : i + 1 \mapsto i \mod n
\]

Thus we get

\[
Z_n[A] \propto \prod_{i=1}^{n_A} \mathcal{T}_n(u_i, 0)\tilde{\mathcal{T}}_n(v_i, 0) \quad \text{with} \quad A = \bigcup_{i=1}^{n_A} [u_i, v_i] : (1.45)
\]

for \( x \in A_j \equiv [u_j, v_j] \), consecutive copies are connected through \( \tau = 0 \) due to the presence of the cut produced by \( \mathcal{T}_n(u_j, 0) \) while, for \( x \notin A \), the effects of \( \mathcal{T}_n(u_j, 0) \) and \( \tilde{\mathcal{T}}_n(v_j, 0) \) cancel each other for any \( j \) such that \( v_j < x \), and the copies are connected to themselves through \( \tau = 0 \). In general, if \( \hat{O}(x, \tau; i) \) is a field lying on the \( i \)th sheet of the Riemann surface \( \mathcal{R}_n[A] \), then we have

\[
\langle \hat{O}(x, \tau; i) \cdots \rangle_{\mathcal{L}[\varphi];\mathcal{R}_n[A]} = \frac{\langle \prod_{i=1}^{n_A} \mathcal{T}_n(u_i, 0)\tilde{\mathcal{T}}_n(v_i, 0)\hat{O}_i(x, \tau) \cdots \rangle_{\mathcal{L}[\varphi];\mathcal{R}_n[A]}}{\langle \prod_{i=1}^{n_A} \mathcal{T}_n(u_i, 0)\tilde{\mathcal{T}}_n(v_i, 0) \rangle_{\mathcal{L}[\varphi];\mathcal{R}_n[A]}}
\]

where \( \hat{O}_i \) is the corresponding field in the model formed by \( n \) independent copies, coming from the \( i \)th copy of \( \mathcal{L} \).

Because the Rényi entropies with integral index (remind, \( n \) is the number of sheets) can be written as (cf. Eq. (1.30))

\[
S_n = \frac{\log \text{Tr} \rho_A^n}{1 - n} = \frac{\log Z_n[A]}{1 - n} + \frac{n}{n - 1} \log Z,
\]

where \( Z \) does not depend on \( A \), we finally get

\[
S_n = \frac{\log \langle \prod_{i=1}^{n_A} \mathcal{T}_n(u_i, 0)\tilde{\mathcal{T}}_n(v_i, 0) \rangle}{1 - n} + c_n',
\]

where \( c_n' \) is a non universal constant. Although Eq. (1.48) is correct only for integral values of \( n \), if a unique proper analytic continuation of \( S_n \) exists, we can extract the entanglement
1. ENTANGLEMENT ENTROPIES: AN OVERVIEW

entropy by exploiting the relations \[1.7\] or \[1.8\]. This procedure is commonly called ‘replica trick’ and is employed successfully in many situations.

In the paragraph below we apply the result \[1.48\] to a conformal system in the special case of a single interval \(n_A = 1\). Indeed the conformal invariance fixes completely the functional dependence on the distance of the two-point correlation function. The case of two disjoint intervals is very complicated, and we refer the interested reader to the papers [14, 27]. It is worth noting that, up to now, it has not been possible to use the ‘replica trick’ in order to extract the entanglement entropy of disjoint blocks: the entanglement entropy of two disjoint intervals is still an open question.

**Entanglement entropy in CFT.** The entanglement entropy of an interval in a CFT has been calculated for the first time in [21]. In [5] the Rényi entropies have been re-derived (and written explicitly), and the previous results have been generalized to finite temperatures, finite lengths, and systems with boundaries.

Here we consider the simplest case of an interval \(A\) at temperature zero. We express the fields in terms of the complex variables \(w = x + i \tau\) and \(\bar{w} = x - i \tau\), where \(x\) is the position and \(\tau\) is the imaginary time, as in the previous section. By indicating the subsystem’s boundaries with \(u\) and \(v\) (\(A = [u, v]\)), the conformal mapping \(w \to \zeta = \frac{w - u}{w - v}\) maps the branch points to \((0, \infty)\). The further transformation \(\zeta \to z = \zeta^{\frac{1}{n}} = \left(\frac{w - v}{w - u}\right)^\frac{1}{n}\) maps the whole of the \(n\)-sheeted Riemann surface \(\mathcal{R}_n[A]\) to the \(z\)-plane \(\mathbb{C}\). We consider the holomorphic component of the stress tensor \(T(w)\). Because the stress tensor transforms as \[7, 37\]

\[
T(w) = \left(\frac{dz}{dw}\right)T(z) + \frac{c}{12} \{z, w\},
\]

where \(c\) is the central charge of the CFT and

\[
\{z, w\} \equiv \frac{d^2z}{dw^2} - \frac{3}{2} \left(\frac{dz}{dw}\right)^2 \frac{d^2w}{dz^2}.
\]

is the Schwarzian derivative, the expectation value of the stress tensor defined in \(\mathcal{R}_n[A]\) can be easily expressed in terms of the stress tensor in \(\mathbb{C}\). In fact \(\langle T(z) \rangle_{\mathbb{C}} = 0\), by translation and rotation invariance, hence we find

\[
\langle T(z) \rangle_{\mathcal{R}_n[A]} = \frac{c(1 - n^2)}{24} \frac{(v - u)^2}{(w - u)^2(w - v)^2}.
\]

Eq. \[1.46\] can be used to write the correlation functions in the \(n\)-sheeted Riemann surface \(\mathcal{R}_n[A]\) in terms of correlation functions in the model formed by \(n\) independent copies. In fact this latter model is a CFT with stress tensor \(T^{(n)}(w) = \sum_{j=1}^n T_j(w)\), where \(T_j(w)\) is the stress tensor of the \(j^{th}\) copy of the Lagrangian \(\mathcal{L}\). In particular the central charge is \(n\) times that of \(\mathcal{L}\). Finally we get

\[
\frac{\langle T_n(u, 0)T_n(v, 0)T^{(n)}(w) \rangle_{\mathcal{L}}}{\langle T_n(u, 0)T_n(v, 0) \rangle_{\mathcal{L}}} = n \langle T(z) \rangle_{\mathcal{R}_n[A]} = \frac{c(n^2 - 1)}{24n} \frac{(v - u)^2}{(w - u)^2(w - v)^2}.
\]
1.2 Entanglement entropies in the ground state of quantum spin chains

This equation must be compared with the Ward identity corresponding to the insertion of the stress tensor \[\mathcal{T}\], which for our two-point correlation function reads as

\[
\langle \mathcal{T}_n(u,0) \tilde{\mathcal{T}}_n(v,0) \rangle_{\mathcal{C},c} = \left( \frac{1}{w-u} \frac{\partial}{\partial u} + \frac{h_n}{(w-u)^2} + \frac{1}{w-v} \frac{\partial}{\partial v} + \frac{\tilde{h}_n}{(w-v)^2} \right) \langle \mathcal{T}_n(u,0) \tilde{\mathcal{T}}_n(v,0) \rangle_{\mathcal{C},c}, \tag{1.53}
\]

where \( h_n \) and \( \tilde{h}_n \) are the scaling dimensions of the primary twist fields \( \mathcal{T}_n \) and \( \tilde{\mathcal{T}}_n \). Thus we find that \( \mathcal{T}_n \) and \( \tilde{\mathcal{T}}_n \) have the same scaling dimension

\[
h_n = \tilde{h}_n = c_{12} \left( \frac{n}{n-1} \right), \tag{1.54}
\]

where we used that conformal invariance fixes the functional dependence of the two-point correlation function

\[
\langle \mathcal{T}_n(u,0) \tilde{\mathcal{T}}_n(v,0) \rangle_{\mathcal{C},c} = (v-u)^{-2h_n}. \tag{1.55}
\]

Inserting Eq. (1.55) into Eq. (1.48) we get the Rényi entropies of an interval \( A \) in a conformal system

\[
S_n[A] = \frac{c}{6} \frac{1+\frac{n}{n}}{n} \log \frac{\ell_A}{a} + c'_n, \tag{1.56}
\]

where \( a \) is a renormalization constant (the lattice spacing of the chain, for instance) which makes the result dimensionless. The analytic continuation is straightforward and the replica trick works: by taking the limit as \( n \to 0^+ \) we obtain the celebrated formula for the entanglement entropy of an interval in a CFT

\[
S_{v.N.}[A] = \frac{c}{3} \log \frac{\ell_A}{a} + c'_1. \tag{1.57}
\]

We conclude this section observing that, because \( Z_n[A] \) transforms as the two-point function of two primary fields, the entanglement entropies of an interval in a conformal system at finite temperature \( \beta^{-1} \) can be obtained by exploiting the conformal mapping \( w \to z = \frac{\beta}{\pi} \log w \) (we need to map the plane into the strip \( \tau \in (0, \beta) \)). The same mapping, with \( L \) instead of \( \beta \), gives the entropies of a subsystem in the ground state of a periodic one dimensional system, \( L \) in length, that is conformal in the thermodynamic limit \( L \to \infty \). In particular for finite lengths (but the result for finite temperatures is the same, provided to substitute \( L \) with \( \beta \)) the entanglement entropies can be obtained by replacing the subsystem’s length \( \ell_A \) with the chord length

\[
\ell_A \to \frac{L}{\pi} \sin \left( \frac{\pi \ell_A}{L} \right), \tag{1.58}
\]

i.e.

\[
S_n[A] = \frac{c}{6} \frac{1+\frac{n}{n}}{n} \log \left| \frac{L}{\pi} \sin \left( \frac{\pi \ell_A}{L} \right) \right| + c'_n. \tag{1.59}
\]

In Chapter 4 dedicated to the corrections to the scaling, we’ll find that this substitution is indeed sufficient to generalize to finite lengths the corrections to the scaling. However, we’ll
1. ENTANGLEMENT ENTROPIES: AN OVERVIEW

find oscillatory factors multiplying the power-law corrections that have periods of the order of
the lattice spacing \( a \): they are not scaling terms and remain independent of the system's length.

In the section below we consider a completely different situation. Contrary to conformal
field theories, in which the behavior of the entanglement entropies can be seen as the manifest-
ation of the system’s symmetries, in random quantum systems the randomness introduced
in the Hamiltonian breaks the symmetries, that are eventually (but only partially: conformal
symmetry remains broken) recovered only after taking the disorder average.

1.2.2 Random quantum systems

The most celebrated example of phases induced by disorder is without doubt the phenomenon
of Anderson localization \[38\]: the wavefunction of quantum particles moving in a spatially
random potential can become localized, as a sufficiently strong disorder is introduced.

However, here we consider a class of systems that, introducing randomness in the Hamilto-
nian, undergo a different phase transition, in which disorder drives the system to the so-called
random-singlet phase. This is the resulting phase of the random spin-\( \frac{1}{2} \) Heisenberg chain, as
well as the random \( XXZ \) and \( XX \) chains: at low energies the state consists of pairs of spins
which are coupled together into singlets over arbitrary long distances. Most of spins pair with
nearby ones, but pairs between arbitrary distant spins appear too. In any case bonds do not
cross each other. Typically, the spin-spin correlations \( C_{ij} \equiv \langle \vec{s}_i \cdot \vec{s}_j \rangle \) decay as follows \[39\]

\[
- \log C_{ij} \sim \sqrt{|i - j|}
\]

However, the disorder averaged correlations \( \overline{C_{ij}} \) are dominated by the rare event of the formation
of a singlet between the sites \( i \) and \( j \), hence the mean correlation decays as the power-law

\[
\overline{C_{ij}} \sim \frac{1}{|i - j|^2}.
\]

Notice that the decay can be faster than in the absence of randomness (e.g. in the pure XX
chain \( C_{ij} \sim |i - j|^{-\frac{1}{2}} \)), and this is due to the completely different underlying physics.

The random-singlet phase belongs to the class of infinite randomness fixed points, which
have well-known scaling properties. They are gapless, but the gap \( \Delta \) does not approach 0 as a
power of the correlation length \( \xi \), as in pure critical points where \( \Delta \sim \xi^{-z} \) (cf. Eq. \[3\]) and
\( z \) is the dynamical exponent. In infinite randomness fixed points another critical exponent \( \psi \)
comes into play, and the scaling law becomes

\[
\Delta \sim e^{-\xi^\psi}
\]

The fundamental critical exponent \( \chi \) of the infinite randomness fixed points is instead related
to the effective distribution of couplings \( P(J) \) that describes the low energy behavior. The
distribution is universal, i.e. independent of the distribution of randomness in the Hamiltonian,
and it is given by

\[
P(J) \sim \frac{1}{J^{1-\frac{1}{\psi}}},
\]
where $\Gamma$ is a parameter that keeps track of the energy scale at which the effective distribution provides a reliable description.

In fact the random-singlet phase is an infinite randomness fixed point with $\psi = \frac{1}{2}$ and $\chi = 1$. In the paragraph below we compute the entanglement entropies averaged over the disorder; here some general features of the RDM and of the entanglement entropies in the random-singlet phase. Because the ground state is a tensor product of singlets, the entanglement of a subsystem has a direct interpretation in terms of the $b_A$ bonds linking the subsystem with the rest. Indeed the reduced density matrix can be written as

$$\rho_A \sim \bigotimes_{i=1}^{b_A} \frac{I_i}{2} \otimes \rho_{in}^{(A)}, \tag{1.64}$$

where $\rho_{in}^{(A)}$ is a pure RDM consisting of the tensor product of the singlets lying in $A$, while $I_i$ is the identity of the space associated to the $i$th spin paired with an external spin. The disorder averaged entanglement entropies are all the same and proportional to the averaged number of bonds over the subsystem’s boundaries

$$S_{\alpha}[A] = \log \frac{\text{Tr} \rho_A^\alpha}{1 - \alpha} = \log 2 \overline{b_A}. \tag{1.65}$$

This is an unusual feature contrasted with the CFT dependence on $\alpha$. In Chapter 6 we will consider the entanglement spectrum in the random-singlet phase, which is instead determined by the full probability distribution of the number of bonds and has a non trivial dependence on the Rényi parameter.

**Random-singlet phase.** As a model, we consider the random XX chain

$$H_{XX} = \frac{1}{4} \sum_l J_l (\sigma_l^x \sigma_{l+1}^x + \sigma_l^y \sigma_{l+1}^y). \tag{1.66}$$

In the absence of randomness ($J_l = J > 0$) the system is conformal with central charge equal to 1. And the entanglement entropies grow with the logarithm of the subsystem’s length, in agreement with Eq. [1.33]. When disorder is introduced, the two spins, coupled through the strongest coupling constant $\Omega = \max_i \{J_i\}$, tend to form a singlet, and the effects of the neighboring couplings can be treated perturbatively. The state can be effectively described by a Hamiltonian in which the two strong coupled spins decouple from the rest

$$H_{XX}^{(1)} = \frac{\Omega}{4} (\sigma_l^x \sigma_{l+1}^x + \sigma_l^y \sigma_{l+1}^y) + \frac{\overline{J}_l}{4} (\sigma_{l-1}^x \sigma_{l+2}^x + \sigma_{l-1}^y \sigma_{l+2}^y) + \frac{1}{4} \sum_{|l-l'|>1} J_l (\sigma_l^x \sigma_{l+1}^x + \sigma_l^y \sigma_{l+1}^y),$$

where (Ma-Dasgupta rule [40][41])

$$\overline{J}_l^{(1)} = \frac{J_{l-1} J_{l+1}}{J_l} \quad (J_l = \Omega) \tag{1.67}$$

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1. ENTANGLEMENT ENTROPIES: AN OVERVIEW

is the effective coupling constant induced by quantum fluctuations, treated within second order perturbation theory. This observation opens the way for an iterative real-space renormalization group approach. Indeed, ignoring the trivial part describing the singlet, the new Hamiltonian has fewer degrees of freedom and the effective interaction between neighboring spins is suppressed $J^{(1)}_i < \Omega$. After many iterations (decimations) more and more distant spins form singlets and, eventually, all spins will have paired in singlets.

The standard way \[39\] to describe this process is by constructing a flow equation for the distribution of couplings. The Ma-Desgupta rule (1.68) becomes linear when expressed in terms of the variables

$$\beta_i = \log \frac{\Omega}{J_i} \quad \text{with} \quad \Omega = \max_i \{J_i\},$$

namely $\tilde{\beta} = \beta_L + \beta_R$, where $L$ and $R$ indicate bonds to the left and to the right of the decimated bond (in fact, the Heisenberg chain is completely equivalent to the XX one, provided that $\Omega$ must be doubled). By indicating with $\Gamma$ the logarithmic RG flow parameter

$$\Gamma = \log \frac{\Omega_0}{\Omega},$$

where $\Omega_0$ is the maximal coupling constant in the original Hamiltonian ($\Gamma \geq 0$ increases under RG flow), the variation in the distribution of bonds resulting from a few of decimations has two sources: the translation in the definition of $\beta_i \equiv \log \frac{\Omega}{J_i} - \Gamma$ and the decimation that the fraction of bonds with $\beta \in (0, \delta \Gamma)$, i.e. $P(0; \Gamma)d\Gamma$, undergo

$$(dP_{\Gamma+\delta\Gamma})(\beta) = (dP_{\Gamma})(\beta) + \delta \Gamma P(0; \Gamma) \int (dP_{\Gamma})(\beta_L) \int (dP_{\Gamma})(\beta_R) d\beta \delta(\beta - \beta_L - \beta_R),$$

where $(dP_{\Gamma})(\beta) \equiv P(\beta; \Gamma)d\beta$ is the probability of the coupling $\beta$ at the RG scale $\Gamma$. In differential form the flow equation reads as

$$\frac{\partial}{\partial \Gamma} P(\beta; \Gamma) = \frac{\partial}{\partial \beta} P(\beta; \Gamma) + P(0; \Gamma) P_{\Gamma} B_{\Gamma},$$

where we introduced the notation

$$A_{\Gamma} \times B_{\Gamma} \equiv \int_0^\infty d\beta_L A(\beta_L; \Gamma) \int_0^\infty d\beta_R B(\beta_R; \Gamma) \delta(\beta - \beta_L - \beta_R).$$

The fixed points of the flow equation above have been studied by Fisher in \[39\], which found a one-parameter family of solutions in which the distribution is singular at small $J$ and the low-energy behavior is dominated by the weakest links. However, he also found a special stable fixed point

$$P(\beta, \Gamma) = \frac{1}{\Gamma} e^{-2 \chi},$$

corresponding to the distribution (1.63) with $\chi = 1$. This distribution is the key to physical characteristic of the random-singlet phase. For example from Eq. (1.74) it follows that the critical exponent $\psi$ (cf. Eq. (1.62)) is equal to $\frac{1}{2}$.

---

1At the first order in the variation of $\Gamma$, just consecutive spins pair in singlets.
1.2 Entanglement entropies in the ground state of quantum spin chains

In order to get the entanglement entropies we need the disorder average of the number of bonds $b_A$ linking the subsystem with the rest (see Ref. [42] for a review on entanglement in random quantum systems). The first step is to construct a flow equation for the strength distribution $Q(\beta, \Gamma)$ of the effective bond, once fixed the link. For example, from (1.71) it follows that, initially, $dQ_\Gamma$ is the conditional probability of the effective bond, given the occurrence of a decimation, i.e.

$$
(dQ_\Gamma)(\beta) = \int (dP_\Gamma)(\beta_L) \int (dP_\Gamma)(\beta_R) \ d\beta \delta(\beta - \beta_L - \beta_R).
$$

(1.75)

Because of the Ma-Desgupta rule (1.68), the probability of having two (consecutive) decimations at the same link is strongly suppressed with respect to the probability of a decimation at the neighboring links, hence we can neglect it. This means that the strength of the effective bond can change only if two neighboring spins pair in a singlet, i.e.

$$
(dQ_{\Gamma+\delta\Gamma})(\beta) = (dQ_\Gamma)(\beta) + 2 P(0; \Gamma) \left[ Q_\Gamma^\beta - Q(\beta; \Gamma) \right].
$$

(1.76)

where the first term on the r.h.s. is again due to the change (translation) in the definition of $\beta$. The factor 2 in front of the second term takes into account that the decimation can occur to the left or to the right. The term in square bracket is the conditional probability of the effective bond, given the occurrence of a decimation in the neighborhoods of the bond; clearly, the strength probability before the decimation must be subtracted. In differential form Eq. (1.76) with the boundary condition (1.75) can be written as [42]

$$
\frac{\partial}{\partial \Gamma} Q(\beta; \Gamma) = \frac{\partial}{\partial \beta} Q(\beta; \Gamma) + 2 P(0; \Gamma) \left[ P_\Gamma^\beta \times Q_\Gamma - (dQ_\Gamma)(\beta) \right]
$$

(1.77)

We got Eq. (1.76) (and so Eq. (1.77)) by neglecting the probability of two decimations over the same bond, hence $p_\Gamma \equiv \int_0^\infty d\beta Q(\beta; \Gamma)$ is the probability that the bond has not been decimated again. Notice that, by integrating out $\beta$ in Eq. (1.77)

$$
\frac{dP_\Gamma}{d\Gamma} = -Q(0; \Gamma),
$$

(1.78)

d$\Gamma Q(0, \Gamma)$ turns out to be the probability of “waiting RG time” after a decimation. The flow equation (1.77) can be solved easily using the ansatz $Q(\beta, \Gamma) = (a_\Gamma + b_\Gamma \beta) P(\beta; \Gamma)$. Eventually we get

$$
d\Gamma Q(0, \Gamma) = d\Gamma a_\Gamma P(0; \Gamma) = d\mu e^{-\frac{3\sqrt{2}}{2} \mu} - e^{-\frac{3+3\sqrt{2}}{2} \mu},
$$

(1.79)

where we introduced the RG time $\mu = \log \frac{\Gamma}{\Gamma_0}$. We expect that the averaged number of singlets over the bond $\tau$ would be a functional of the probability $d\Gamma Q(0, \Gamma)$, independent explicitly of $\Gamma$ and $\Gamma_0$. This means that it is a function of the RG time $\mu$ alone. From these observations we get the following renewal equation

$$
\pi_{(\mu)} = \int_0^\mu d\tau \pi_{(\mu)} e^{\tau} Q(0; e^{\tau} \Gamma_0) (1 + \pi_{(\mu - \tau)})
$$

(1.80)
This can be easily solved in Laplace transform, indeed

$$\pi(\mu) = \mathcal{L}^{-1}\left[\frac{\hat{Q}(0, s)}{s(1 - Q(0, s))}\right](\mu) \sim \frac{\mu}{\int_{\Gamma_0} \mathrm{d}\Gamma \log \left(\frac{\Gamma}{\Gamma_0}\right) Q(0, \Gamma)} + O(\mu^0),$$

(1.81)

where

$$\hat{Q}(0, s) = \int_{\Gamma_0}^\infty \mathrm{d}\Gamma \left(\frac{\Gamma_0}{\Gamma}\right)^s Q(0, \Gamma) = \int_0^\infty \mathrm{d}\tau \frac{e^{-\frac{3-\sqrt{5}}{2}\tau} - e^{\frac{3-\sqrt{5}}{2}\tau}}{\sqrt{5}} = 3,$$

(1.82)

and we extracted the leading behavior from the pole in $s = 0$ (notice that $Q$ is normalized, namely $\int_{\Gamma_0}^\infty \mathrm{d}\Gamma Q(0, \Gamma) = 1$). Thus we found $\pi(\mu) = \frac{\mu}{4}$. The final step is to express the RG time $\mu$ in terms of the subsystem’s length $\ell_A$. In fact the averaged length of bonds behaves as $\bar{\ell} \sim \Gamma^{1/\psi} = \Gamma^{2}$ [39], but only the bonds up to the length scale $\ell_A$ can contribute to the entanglement entropy of $A$, hence we expect the scaling law $\ell_A \sim \Gamma^2 = e^{2\mu \Gamma_0^2}$. Because the interval $A$ has two boundaries, the r.h.s. of Eq. (1.81) must be multiplied by 2. Finally, the entanglement entropies have the typical logarithmic growth observed in critical systems

$$S_\alpha[A] = \log 2b_A = \log 2^{\frac{2}{3}}\mu \sim \log 2^{\frac{2}{3}} \log \ell_A,$$

(1.83)

which generalizes to

$$S_\alpha[A] \sim \frac{\log 2c}{3} \log \ell_A$$

(1.84)

when the corresponding pure system is conformal with central charge $c$. Many speculative attempts have been made at interpreting $c \log 2$ has an effective central charge. However we stress that such interpretations are completely meaningless, considering that the Rényi entropies in the random-singlet phase are independent of the Rényi parameter $\alpha$, while in conformal systems they have the exact dependence \(1.33\).

In this chapter we overviewed the most important features of Rényi entropies and, in particular, of the entanglement entropy. We discussed in rather detail strong subadditivity, which is the peculiar property of the entanglement entropy, and we analyzed its effects on the dependence of the entropy on the subsystem’s geometry and system’s boundary conditions. We gave an outline of the behavior of the entanglement entropies of connected subsystems in the ground state of quantum spin chains, considering two typical examples of critical systems: conformal and random quantum systems. We sketched out the proofs of the formulae for the entanglement entropies of an interval both in a CFT and in a random system driven in the random-singlet phase.
2. Exactly solvable spin chains

The importance of the spin interaction $\vec{S}_i \cdot \vec{S}_j$ traces back to the Heisenberg and Dirac’s works [44][45], where they found it arises naturally as an effective interaction between electrons in neighboring atoms. In particular, they discovered that such interaction could explain the phenomenon of ferromagnetism, and indeed spin interaction was soon recognized as the key to a microscopic description of ferromagnetism. Not many years later, in 1931 Hans Bethe presented the first exact solution of a many-body quantum system [46], namely the spin-$\frac{1}{2}$ Heisenberg model, which is a chain of spins with interaction between nearest neighbors. Bethe constructed the many-body wave functions and reduced the problem of calculating the spectrum of the Hamiltonian to an algebraic one. His work has influenced the research in mathematical and theoretical physics to an extent not imagined at the time, and can be considered the beginning of a new branch of physics, the theory of exactly solvable models.

The importance of exactly solvable models is twofold: on the one hand the availability of analytical and exact numerical results can be used to extract universal features, common to all systems in the same universality class; on the other hand, the connection between models solved by Bethe ansatz and integrability (roughly speaking, the existence of infinite conservation laws) opens the way for a deeper understanding of the meaning and implications of integrability in quantum mechanics. In fact such connection has been established in 1979, when Fadeev, Sklyanin, and Takhtadzhyan [47][48] formulated the quantum method of the inverse scattering problem, which includes an algebraic version of the Bethe ansatz. Models with quite heterogeneous physical content can be described in that framework, corresponding different quantum systems to different representations of the algebra. This expresses the universality of the algebraic approach, in contrast to the embryonic method proposed initially by Bethe, very model-dependent and, because of the complicated structure of eigenvectors, generally unsuitable for computing correlation functions. The algebraic Bethe ansatz allows to construct the eigenfunctions of several physical models in a unified way, but one still faces with several difficulties. Indeed, the algebraic Bethe ansatz is based on the algebra of operators of the so-called monodromy matrix, which turns out to be a non-local algebra. For this reason, it is anything but straightforward the inclusion of the local operators of the original model (in order to compute correlation functions, for instance) and, also when this problem can be overcome
2. EXACTLY SOLVABLE SPIN CHAINS

(e.g. in Heisenberg spin chains), the commutation relations are complicated insomuch that the answers provided by the algebraic Bethe ansatz can be useless, in practice.

In the next paragraph, we provide a concise account of the Bethe ansatz solution of the Heisenberg model. In the rest of the work, however, we will not consider models solvable in the sense of Bethe ansatz. The physical aspects we are interested in, namely the entanglement properties and some aspects of quench dynamics, do not generally find a helpful ground in the framework of (algebraic) Bethe ansatz. In fact, the paragraph is intended as a guide to distinguish the features that are typical of integrable models from those specific of models that can be mapped into non-interacting fermion systems, which instead will be studied extensively.

Bethe ansatz: the Heisenberg model. The Heisenberg model (XXX chain) is a periodic chain of spin-$\frac{1}{2}$ particles, which interact between nearest neighbors. It is described by the Hamiltonian

$$H = -J \sum_{n=1}^{L} \vec{S}_n \cdot \vec{S}_{n+1} \quad \left( = \frac{3JL}{4} - \frac{J}{2} \sum_{n=1}^{L} |\vec{S}_n + \vec{S}_{n+1}|^2 \right),$$

where $\vec{S}_n$ is the spin operator in the $n^{th}$ site and $J$ is the coupling constant. Periodic boundary conditions $\vec{S}_{L+1} \equiv \vec{S}_1$ are understood. We assume $L$ divisible by 4. If $J > 0$ the model is ferromagnetic, otherwise it is antiferromagnetic. For the sake of simplicity we consider the ferromagnetic Heisenberg model. The Hamiltonian is rotational invariant but the ground state $|\Psi_0\rangle$ spontaneously breaks the symmetry, so that all spins are aligned in the same direction $|\Psi_0\rangle = |\uparrow \cdots \uparrow\rangle$ and the energy is equal to $E_0 \equiv -\frac{JL}{4}$.

Because the Hamiltonian commutes with the total spin $S^z = \sum_{n=1}^{L} S^z_n$, it can be block diagonalized by fixing $S^z = \frac{L}{2} - r$, where $r$ is the number of down spins. For a given $r$, the eigenfunctions can be written as

$$|\Psi\rangle = \sum_{1 \leq n_1 < \cdots < n_r \leq L} a(n_1, \ldots, n_r) S^-_{n_1} \cdots S^-_{n_r} |\Psi_0\rangle,$$

where we indicated with $S^\pm_n \equiv S^z_n \pm i S^y_n$ the spin flip operators. The Bethe ansatz fixes the form of the coefficients $a$ [49]:

$$a(n_1, \ldots, n_r) = \sum_{\pi \in S_r} \exp\left(i \sum_{j=1}^{r} \theta_{\pi,j} n_j + \frac{i}{2} \sum_{i<j} \theta_{\pi,i} \theta_{\pi,j} \right),$$

where $S_r$ denotes the set of permutations of $\{1, \ldots, r\}$. The Schrödinger equation $H |\Psi\rangle = E |\Psi\rangle$ and the constraint of periodicity give the following consistency equations (Bethe ansatz equations):

$$2 \cot \frac{\theta_{ij}}{2} = \cot \frac{k_i}{2} - \cot \frac{k_j}{2}$$

$$k_i = \frac{2\pi \lambda_i}{L} + \frac{1}{L} \sum_{j \neq i}^{r} \theta_{ij} \quad \Rightarrow \quad i = 1, \ldots, r,$$

where $\lambda_i$ are the roots of the Bethe ansatz equations.
where $\lambda_i \in \{0, 1, \ldots, L - 1\}$ are the so-called Bethe quantum numbers. Finally, every solution represents an eigenvector with energy and wave number given by

$$E - E_0 = 2J \sum_{j=1}^{r} \sin ^2 \left( \frac{k_j}{2} \right) \quad k \equiv \sum_{i=1}^{r} k_i = \frac{2\pi}{L} \sum_{i=1}^{r} \lambda_i .$$ \hspace{1cm} (2.5)$$

We analyze in more details the sectors $r = 1, 2$, in order to show how Bethe ansatz helps to organize the states depending on their physical properties [49]. The Bethe equations for $r = 1$ are trivial, indeed they are solved by $k = \frac{2\pi m}{L}$ where $m \in \{0, \ldots, L - 1\}$. The eigenstates

$$|\psi_m \rangle = \frac{1}{\sqrt{L}} \sum_{l=1}^{L} e^{2\pi i ml} \bigg| \overbrace{\uparrow \cdots \uparrow}^{l-1} \downarrow \cdots \downarrow \bigg|_{L-l} \quad m = 0, \ldots, L - 1$$ \hspace{1cm} (2.6)$$

represent the so-called magnon excitations, in which the ground state is perturbed by spin waves. The energy of the excitations is given by

$$E_m - E_0 = 2J \sin ^2 \left( \frac{\pi m}{L} \right).$$ \hspace{1cm} (2.7)$$

The interesting physics comes into play considering the sector $r = 2$. Not all pairs $(\lambda_1, \lambda_2)$ of Bethe quantum numbers solve the Bethe equations [2.4] for some $\theta$’s, indeed there are $\frac{L(L-1)}{2}$ solutions, while there are $\frac{L(L+1)}{2}$ ordered pairs of $(\lambda_1, \lambda_2)$. The solutions can be grouped into three classes, according to the values of $(\lambda_1, \lambda_2)$:

1. $(0, \lambda_2)$ for any $\lambda_2 \in \{0, \ldots, L - 1\}$; they have the same dispersion relation as the magnon excitations in the sector $r = 1$. They can be interpreted as exact superpositions of a magnon with momentum zero and another magnon with a given momentum.

2. $(\lambda_1, \lambda_2)$ with $\lambda_2 > \lambda_1 + 2 > 2$; the momenta that solve the Bethe equations are real. They can be seen as two-magnon scattering states, being the excitation energy of the two-magnon states modified by the magnon interaction. As the chain’s length increases, however, the energy correction due to the interaction decreases, until vanishing in the thermodynamic limit $L \rightarrow \infty$. Thus, in the continuum limit they become free two-magnon states.

3. $(\lambda_1, \lambda_2)$ with $|2(\lambda_2 - \lambda_1) - 1| = 1$; the Bethe equations are solved by complex (conjugate) momenta for $\lambda_2 = \lambda_1$ and $|\lambda_1 - \frac{L}{2}| = \frac{L}{4} + 1, \ldots, \frac{L}{2} - 1$, as well as for $\lambda_2 = \lambda_1 + 1$ and $|\lambda_1 - \frac{L}{2}| = \frac{L}{4} + 1, \ldots, \frac{L-1}{2} - 1$, where $\lambda \sim \sqrt{L}$. The solutions are real for $\lambda_2 = \lambda_1 + 1$ and $|\lambda_1 - \frac{L-1}{2}| = \frac{L+2-\lambda}{2}, \ldots, \frac{L-3}{2}$. For $\lambda_2 = \lambda_1 = \frac{L}{4}$ there is a solution, corresponding to $k = \pi$, in which the momenta have infinite imaginary part. In contrast to the second class of states, described above, here the effects of the magnon interaction survive the continuum limit. In fact these states have a dispersion relation below the continuum of two-magnon scattering states: they are bound states. The probability amplifies as the two flipped spins come closer and it is peaked at one lattice spacing.
2. EXACTLY SOLVABLE SPIN CHAINS

The generalization to higher values of \( r \) reveals a fundamental feature of (algebraic) Bethe ansatz: the scattering between many quasi-particles can be traced back to the scattering between pairs of them (the phase angles \( \theta \) have two indices). This is eventually due to the existence of many conservation laws (charges), whose underlying symmetries allow to factorize the \( n \)-body scattering-matrix into a sequence of 2-body ones.

In conclusion, the Bethe ansatz provides a very useful classification of the stationary states, uncovering the physical properties of the excitations. Scattering states and bound states, as well as the nature of excitations, arise naturally. Incidentally, the latter could be better understood in the framework of algebraic Bethe ansatz, where eigenfunctions are created by creation and annihilation operators acting on a pseudovacuum.

The possibility to solve the model by means of (algebraic) Bethe ansatz is related to the concept of integrability. A classical system with a 2\( n \)-dimensional phase space, e.g. a system of \( n \) classical spins, is integrable if it has \( n \) independent integrals of motion (analytic invariants) \( I_j \) in involution, i.e. with vanishing Poisson brackets between each other \[50\]. In particular the Poisson brackets between spin components are defined as

\[
\{ S_{n,\alpha}, S_{n',\beta} \} = -\delta_{nn'} \sum_{\gamma=x,y,z} \varepsilon_{\alpha\beta\gamma} S_{n,\gamma},
\]

with \( \varepsilon \) the Levi-Civita symbol. Analyticity guarantees that \( \{ H, I_j \} \) is well-defined. Independence means that the directions \( \nabla I_j \) are linearly independent almost everywhere in phase space. The definition of an integrable quantum system is instead much less clear: we cannot ask just for the existence of \( n \) independent commuting operators because we would fail to state which operators should be counted and what makes two operators independent. Generally, a quantum system with an integrable classical limit is said to be integrable, but also models exactly solvable by algebraic Bethe ansatz are called integrable. These ambiguities rely essentially in the difficulty to discriminate between commuting operators that have a bearing on the question of integrability and those that do not. And, to overcome these problems, in Ref. \[51\] a definition independent of any classical concept has been proposed: integrability is traced back to the existence of a unitary transformation that converts the spin operators into new spin operators such that the Hamiltonians turns into a function of a single component, e.g. the \( z \) component, of the new operators \( H(S_1,\ldots,S_n) \rightarrow \tilde{H}(\tilde{S}_z^1,\ldots,\tilde{S}_z^n) \). While this picture can be useful considering systems of a few spins, it is completely unsuitable for characterizing integrability in many-body quantum systems. The problem of defining integrability in quantum mechanics, and in particular in extended quantum systems, is subtle \[52\] and degeneracy plays an important role. In fact, it is observed that, except for some extraordinary cases, the (energy) level-spacing in integrable systems turns out to be Poisson distributed\[53\], while the typical level-spacing distribution

\[1\] This was first conjectured by Berry and Tabor \[53\], who observed that the spectral fluctuations in the semiclassical limit are well-described by the Poisson statistics. Actually, this is not always true and, for example, the harmonic oscillator does belong to a separate class of integrable systems, being the level-spacing distribution a Dirac-delta function.
for a non-integrable system is the Wigner distribution \[54\] (actually, non-Wigner distributions have been also observed \[55\]). The Poisson distribution is a decreasing function, and hence maximal at level-spacing zero (corresponding to degenerate levels), whereas the Wigner distribution is peaked at a non-zero value of level-spacing, vanishing as the level-spacing approaches zero. This means that, in general, Hamiltonians of integrable systems have highly degenerate levels in contrast to the almost non-degenerate Hamiltonians of non-integrable models.

Confining ourself to spin chains, in which spins interact between nearest-neighbors, in Ref. \[56\] integrability has been put in relation to the existence of a set of local conservation laws, \textit{i.e.} operators in which the interaction involving a certain set of sites disappears when the distances between them become sufficiently large. And in the rest of the work we shall adopt this point of view, \textit{i.e.} we assume that a 1D integrable quantum system has a set of as many (somehow local) commuting Hermitian operators as quantum degrees of freedom, and the Hamiltonian can be expressed as a function of these operators. In chapter \[7\] we will see that quantum integrable systems behave very differently from non-integrable ones when the system is put out of equilibrium. In particular, the existence of infinite local conservation laws is crucial to understand the large time behavior.

The rest of the chapter is devoted to the presentation of the XY model, which we will use in the remainder as the theoretical laboratory for testing the CFT results, as well as “source of inspiration” for the problems that have not been yet solved.

### 2.1 XY model: the paradigm of “non-interacting” chains

The XY model is a spin-\(\frac{1}{2}\) chain described by the Hamiltonian

\[
H_{XY} = -J \sum_{l=1}^{L} \left( \frac{1 + \gamma}{4} \sigma_{l}^{x} \sigma_{l+1}^{x} + \frac{1 - \gamma}{4} \sigma_{l}^{y} \sigma_{l+1}^{y} \right) - \frac{h}{2} \sum_{l=1}^{L} \sigma_{l}^{z},
\]

(2.9)

where \(\sigma_{l}^{\alpha}\) (\(\alpha = x, y, z\)) are the Pauli matrices. \(J\) is the coupling constant, which can be set equal to \(\pm 1\), \(h\) is the transverse magnetic field, and \(\gamma\) is usually called anisotropy constant, encoding the x-y anisotropy of the interaction between neighboring spins. The Pauli matrices \(\sigma_{l+1}^{z}\) must be interpreted as \(\sigma_{l}^{z}\) or \(\emptyset\), depending whether the boundary conditions are periodic (PBC) or open (OBC). In contrast to the Heisenberg model, in which the sign of the coupling constant distinguishes the ferromagnetic model from the antiferromagnetic one, the sign of \(J\) in the XY model is irrelevant. Indeed the transformation

\[
P_{J} \equiv \prod_{l=1}^{\lfloor L/2 \rfloor} \sigma_{2l-1}^{z}
\]

(2.10)

changes the sign of the coupling constant \(J\). Analogously, the transformation

\[
P_{h} \equiv \prod_{l=1}^{L} \sigma_{l}^{z}
\]

(2.11)
inverts the sign of the magnetic field. Because of this, \( J \) can be chosen equal to 1 and \( h \geq 0 \). When \( \gamma = 0 \), the XY model is called isotropic, or XX model; it is gapless for \( h \leq 1 \), and for magnetic fields strictly less than 1 it is conformal with central charge \( c = 1 \). The XY model is also critical in the entire line \( h = 1 \) where, for \( \gamma \neq 0 \), it is conformal with central charge equal to \( \frac{1}{2} \).

In the paragraphs below we provide a qualitative description of two well-known models, included in the XY model: the Ising model and the XX model.

**Ising model.** The quantum Ising model is obtained by setting \( \gamma = 1 \) in the XY Hamiltonian (2.9)

\[
H_{\text{Ising}} = -\frac{J}{2} \sum_{l=1}^{L} \sigma_l^x \sigma_{l+1}^x - \frac{h}{2} \sum_{l=1}^{L} \sigma_l^z ,
\]

and it is the crucial paradigm for quantum critical behavior [6]. In fact, in the thermodynamic limit \( L \to \infty \), the ground state of the Ising Hamiltonian exhibits a second-order quantum phase transition as the magnetic field is tuned across the critical value \( h_c = 1 \). The existence of a critical point can be understood heuristically. In absence of magnetic field, there are two degenerate ferromagnetic ordered ground states: all spins are aligned in the same direction and the two states can be distinguished by the two possible orientations

\[
\langle \rightarrow | \sigma_x | \rightarrow \rangle = 1 \quad \langle \leftarrow | \sigma_x | \leftarrow \rangle = -1 .
\]

The ferromagnetic behavior survives also for weak magnetic fields (actually, the system is ferromagnetic for any \( h < 1 \)), indeed the quantum tunneling between the two states is exponentially small in \( L \) so that the discrete symmetry remains broken. On the other hand, for large magnetic fields \( (h \gg 1) \) the ground state is non-degenerate, being all spins almost aligned in the \( z \) direction \( \langle \sigma_z \rangle \ll 1 \). Moreover, the character of the excitations in the two regions \( h \ll 1 \) and \( h \gg 1 \) is different. The first excited states for weak magnetic fields are domain walls between regions of opposite \( x \)-magnetization

\[
| \rightarrow \cdots \rightarrow \leftarrow \cdots \rangle .
\]

Instead, for strong magnetic fields the excitations are similar to the one-magnon excitations of the ferromagnetic Heisenberg model (cf. [2.6]).

The different physical properties characterizing the two regimes \( h \ll 1 \) and \( h \gg 1 \) suggest that the ground state can not change smoothly as a function of the magnetic field. In fact, the point of non analyticity \( h = 1 \) corresponds to a second-order quantum phase transition, separating the ferromagnetic phase \( h < 1 \) from the paramagnetic one \( h > 1 \). It is described by a CFT with central charge \( c = \frac{1}{2} \).
XX model. The XX model (Eq. (2.9) with $\gamma = 0$)
\[ H_{XX} = -\frac{J}{4} \sum_{i=1}^{L} (\sigma^x_i \sigma^x_{i+1} + \sigma^y_i \sigma^y_{i+1}) - \frac{h}{2} \sum_{i=1}^{L} \sigma^z_i \] (2.15)
is the hard-core limit ($U \rightarrow +\infty$) of the one-dimensional Bose-Hubbard model
\[ H_{B.H.} = -\frac{J}{2} \sum_{<ij>} (b_i^\dagger b_j + b_j^\dagger b_i) + \frac{U}{2} \sum_{i} n_i (1 - n_i) + \mu \sum_{i} n_i \quad n_i = b_i^\dagger b_i , \] (2.16)
with $b_i$ spinless bosons, firstly realized experimentally by Greiner et al. in 2002 [57]. The Bose-Hubbard model provides “one of the simplest realizations of a quantum phase transition which does not map onto a previously studied classical phase transition in one higher dimension” [6]. In fact, by tuning the parameter $J$, it undergoes a quantum phase transition between a Mott insulating phase and a superfluid one. The first term is a hopping term that annihilates a particle to create it at a neighboring site. The second term is the interaction. The third term is an external potential, usually interpreted as the chemical potential. When the repulsive interaction $U$ is sufficiently strong, the model can be mapped into the XX chain. Indeed, for $U$ much larger than $J$ and $\mu$, just the second term of the Bose-Hubbard Hamiltonian survives, hence bosons cannot occupy the same site ($n_i$ cannot be larger than 1). The objects with such a hybrid behavior are called hard-core bosons and satisfy the algebra
\[ [b_i, b_j] = 0 \quad [b_i^\dagger, b_j^\dagger] = \delta_{ij} (1 - 2n_i) \quad [b_i, n_j] = \delta_{ij} b_i \quad b_i^2 = 0 \quad n_i^2 = n_i , \] (2.17)
which is equivalent to the algebra of the Pauli matrices, specified by
\[ \sigma^x_i = b_i + b_i^\dagger \quad \sigma^y_i = i(b_i^\dagger - b_i) \quad \sigma^z_i = 1 - 2n_i . \] (2.18)
Finally, the Bose-Hubbard Hamiltonian (2.16) is mapped, by the transformation (2.18), into the XX Hamiltonian (2.15) (up to an additive constant).

Apart from the connection with the Bose-Hubbard model, the importance of the XX model lies in its simplicity but non-triviality. Indeed, many of the existent analytic and exact numerical results about, for example, the entanglement entropies of subsystems have been obtained considering XX chains.

Here some basics features. The total spin in the $z$ direction $\frac{1}{2} \sum_{i=1}^{L} \sigma^z_i$ commutes with the XX Hamiltonian, hence the eigenvectors of the XX model are independent of the magnetic field $h$. For finite $L$, by tuning the parameter $h$, the physical properties of the ground state do not change with continuity, but they are characterized by continuous levels-crossing. However, for strong magnetic fields $h > 1$ the ground state of the XX model has all spins aligned in the $z$ direction. The model is conformal for any value of $h < 1$ with central charge $c = 1$, but it is also critical for $h = 1$, when the dynamical exponent $z$ becomes equal to 2.

Some specific mathematical features that make the XX model the simplest laboratory for studying the entanglement properties of spin chains, as well as the Ising model the paradigm
to describe the out-of-equilibrium dynamics, will be clear in the following chapters. However, most of the significant features of these models can be traced back to the fermionic mapping that we are going to describe.

**Fermionic mapping.** The XY model can be solved exactly by mapping the Hilbert space of \( L \) spins \( \frac{1}{2} \) into the antisymmetric Fock space of \( L \) spinless fermions \([58, 59]\). This is achieved by the Jordan-Wigner (JW) transformation: the creation and annihilation operators acting on the Fock space can be chosen as

\[
\begin{align*}
    c^+_l &= \prod_{j<l} \sigma^z_l \sigma^+_l \quad c_l &= \prod_{j<l} \sigma^z_l \sigma^-_l
\end{align*}
\]  

(2.19)

where \( \sigma^\pm \equiv \sigma_x \pm i \sigma_y \), and the operators satisfy the anticommutation relations

\[
\{c^+_l, c^+_n\} = 0 \quad \{c^+_l, c_n\} = \delta_{ln} \quad \{c_l, c_n\} = 0.
\]  

(2.20)

Because of the string of \( \sigma^z \), the JW transformation is non-local. Notice, however, that in both spin and fermionic representations the degrees of freedom enclosed in the subspace \([1, \ell]\) are mapped into the corresponding subspace. The non-locality of the transformation affects the boundary conditions. Open boundary conditions mean \( c^+_L + 1 = 0 \). On the other hand, the boundary conditions for the Jordan Wigner fermions when the chain is periodic read as

\[
c^+_L \equiv N c^+_1
\]  

(2.21)

with \( N = \prod_{l=1}^L \sigma^z_l = \pm 1 \) the parity of the spins down, i.e. the parity of the number of fermions. In fact, \( N \) commutes with the XY Hamiltonian and divides the Hilbert space in two subspaces, which must be considered separately. From now on, we will use the same symbol \( N \) for characterizing open boundary conditions too, that is to say \( N^{(OBC)} \equiv 0 \). The XY Hamiltonian (2.9), in terms of the JW fermions, is as follows:

\[
H_{XY} = \frac{J}{2} \sum_{l=1}^{L-1} \left( c^+_l c_{l+1} + \gamma c^+_l c^+_l + H.c. \right) + \frac{J N}{2} \left( c^+_L c_1 + \gamma c^+_L c^+_1 + H.c. \right) - h \sum_{l=1}^L c^+_l c_l + \frac{h L}{2}.
\]  

(2.22)

The fact that the Hamiltonian (2.22) is quadratic in some fermionic operators is crucial for the properties of the model: the Hamiltonian can be diagonalized exactly and the correlation functions can be reduced to the expectation values of pairs of fermionic operators (Wick theorem)

\[
\langle \phi_1 \cdots \phi_n \rangle = \sum_{j=2}^n (-1)^j \langle \phi_1 \phi_j \rangle \langle \phi_2 \cdots \phi_{j-1} \phi_{j+1} \cdots \phi_n \rangle,
\]  

(2.23)

where \( \phi_j \)'s are, for example, Majorana fermions \( \{ \phi_j, \phi_k \} = 2 \delta_{kj} \) and \( \phi^+_j = \phi_j \).
The final step is the Bogolioubov transformation, which relies on the following parameterization defined modulo $L.XY$ breaks translational invariance (in the corresponding fermionic space) JW operators when $N = -1$. Periodicity, however, is a useful feature which allows to block-diagonalize the Hamiltonian in Fourier transform, hence it is worth to recover it. Incidentally, if the periodic chain has odd size, periodicity can be recovered by applying the simple unitary transformation $ar{c}_l = (N)^l c_l$, which gives $(ar{c}_{L+1} = \bar{c}_1)$

$$H_{XY}^{(PBC)}[N] = \frac{JN}{2} \sum_{l=1}^{L} (\bar{c}_l^\dagger \bar{c}_{l+1} + \gamma \bar{c}_l^\dagger \bar{c}_{l+1}^\dagger + H.c.) - \hbar \sum_{l=1}^{L} \bar{c}_l^\dagger \bar{c}_l + \frac{\hbar L}{2} \quad \text{with } L \text{ odd.} \quad (2.24)$$

The transformation $\bar{c}_l = e^{\frac{i(N-1)\pi}{2L}} c_l$ makes an analogous work for a generic $L$ \cite{60}, however it breaks translational invariance (in the corresponding fermionic space)

$$H_{XY}^{(PBC)}[N] = \frac{J}{2} \sum_{l=1}^{L} (\bar{c}_l^\dagger \bar{c}_{l+1} + \gamma e^{-\frac{\pi(N-1)\pi}{2L}} e^{-\frac{\pi(N-1)\pi}{2}} \bar{c}_l^\dagger \bar{c}_{l+1}^\dagger + H.c.) - \hbar \sum_{l=1}^{L} \bar{c}_l^\dagger \bar{c}_l + \frac{\hbar L}{2}. \quad (2.25)$$

In discrete Fourier transform $\bar{c}_l = \frac{1}{\sqrt{L}} \sum_{k=1}^{L} e^{\frac{2\pi i k}{L}} \bar{c}_k$, the Hamiltonian (2.25) (and in particular (2.24)) is block diagonal

$$H_{XY}^{(PBC)}[N] = \frac{1}{2} \sum_{k=-N}^{N} \bar{\eta}_k^\dagger \mathcal{H}_k \bar{\eta}_k, \quad (2.26)$$

where $\bar{\eta}_k$ is the row vector $(\bar{c}_k^\dagger \bar{c}_{1-N-k})$, and $\mathcal{H}_k$ is the Hamiltonian restricted to the space of the momenta $\frac{2\pi k}{L}$ and $\frac{L-1-N-2\pi k}{L}$ (notice that the momentum is defined modulo $2\pi$, i.e. $k$ is defined modulo $L$)

$$\mathcal{H}_k \equiv \left[ J \cos \left( \frac{\pi(N-1)}{2L} + \frac{2\pi k}{L} \right) - \hbar \right] \sigma_z - \gamma J \sin \left( \frac{\pi(N-1)}{2L} + \frac{2\pi k}{L} \right) \sigma_y. \quad (2.27)$$

The final step is the Bogolioubov transformation, which relies on the following parameterization

$$\mathcal{H}_k \equiv e^{-i \frac{\pi}{4} \sigma_x \sigma_z} e^{i \frac{\pi}{4} \sigma_y \varepsilon_k}, \quad (2.28)$$

where $\varepsilon_k$ is the dispersion relation and $\theta_k$ the Bogolioubov angle

$$\varepsilon_k = \sqrt{(J \cos(\varphi_k) - \hbar)^2 + \gamma^2 \sin(\varphi_k)} \quad \varphi_k = \frac{2\pi}{L} \left( k + \frac{N-1}{4} \right)$$

$$\cos \theta_k = \frac{J \cos \varphi_k - \hbar}{\varepsilon_k} \quad \sin \theta_k = \frac{\gamma J \sin \varphi_k}{\varepsilon_k}. \quad (2.29)$$

2.1.1 Periodic boundary conditions

The JW transformation maps the XY model (2.9) with periodic boundary conditions into a chain of fermions, which is not periodic when the state corresponds to an odd number of fermions. Indeed the boundary term in the Hamiltonian (2.22) breaks the periodicity of the chain of fermions, which is not periodic when the state corresponds to an odd number of.
The fermions diagonalizing the subspace corresponding to a given \( N \) can be obtained by taking the scalar product between \( \vec{\eta}_k^\dagger \) and the \( \vec{\psi}_k^{(+)} \)’s eigenvector \( \vec{\psi}_{k}^{(+)} \) with positive eigenvalue

\[
 b^\dagger_k \equiv \vec{\eta}_k^\dagger \cdot \vec{\psi}_{k}^{(+)} = \cos \frac{\theta_k}{2} \vec{c}_k^\dagger - i \sin \frac{\theta_k}{2} \vec{c}_{-N-k}^\dagger ,
\]

so that

\[
 H^{(PBC)}_{XY}[N] = \sum_{k=1}^{L} \epsilon_k \left( b^\dagger_k b_k - \frac{1}{2} \right) .
\]

The Hamiltonian (2.25) (and eventually the diagonal one (2.31)) acts, for fixed \( N \), on a Hilbert space of dimension \( 2^L \), but only the eigenstates with the correct value of \( N \) are also eigenstates of the original Hamiltonian

\[
 H^{(PBC)}_{XY} = \frac{1}{2} + \frac{N}{2} H^{(PBC)}_{XY}[+1] + \frac{1}{2} - \frac{N}{2} H^{(PBC)}_{XY}[-1] .
\]

This means, in particular, that the ground state of the XY model with periodic boundary conditions can be the vacuum of the fermions \( b \) with \( N = 1 \), or the first excited state with \( N = -1 \). Actually, the difference between the energies of the vacua corresponding to \( N = 1 \) and \( N = -1 \) is \( O(1/L) \), hence if the system is gapped and the gap \( \Delta \) is much larger than \( 1/L \), then the ground state of the XY model is the vacuum of the operators \( b \) with \( N = 1 \). If, instead, the system is gapless (in the continuum limit) the ground state of the finite system could belong to the subspace with \( N = -1 \).

We are interested in the XY model at temperature zero. According with the observations above, we can ignore the existence of the subspace with \( N = -1 \), since generally the ground state is in the other subspace. Expressing the JW fermions in terms of the Bogolioubov ones

\[
 \begin{pmatrix} c_l^\dagger \\ c_l \end{pmatrix} \overset{N=1}{=} \frac{1}{L} \sum_{k=1}^{L} e^{-\frac{2\pi ikn}{L}} e^{i(\sigma_x \sigma_y)(b^\dagger_k b_k - \frac{1}{2})} ,
\]

where we introduced the Majorana operators

\[
 a_x^n = c_l + c_l^\dagger , \quad a_y^n = i(c_l - c_l^\dagger) ,
\]

satisfying the algebra \( \{ a_x^n , a_x^{n'} \} = 2\delta_{nn'} \delta_{x} \), with \( x, y = x, y \). The correlation matrix defined in Eq. (2.34) is a structured matrix, called block Toeplitz matrix: the \( 2 \times 2 \) blocks of every diagonal are equal. In fact, this is due to translational invariance. Many results about the asymptotic behavior of the determinant of block Toeplitz matrices (and in particular of Toeplitz ones \( T_{in} = T_{n-i} \)) are known [61]; and in the following chapters we will use such results extensively.
2.1 XY model: the paradigm of “non-interacting” chains

XX model. The Hamiltonian of the XX model can be obtained by sending $\gamma$ to 0 in the XY Hamiltonian \((2.22)\)

$$H_{XX} = \frac{J}{2} \sum_{l=1}^{L-1} (c_l^+ c_{l+1} + c_{l+1}^+ c_l) + \frac{JN}{2} (c_L^+ c_1 + c_1^+ c_L) - h \sum_{l=1}^{L} c_l^+ c_l + \frac{hL}{2}, \quad (2.36)$$

hence the number of $c$ fermions is conserved ($\langle c_l c_n \rangle = \langle c_l^+ c_n^+ \rangle = 0$). The ground state is degenerate if the vacuum of the $b$ operators with $N = 1$ (cf. \(2.31\)) is degenerate with the first excited state of the $b$ operators corresponding to $N = -1$, or with the first two-fermion excited state with $N = 1$. The latter situation is possible only if

$$\frac{L}{2\pi} \arccos \left( \frac{h}{J} \right) \in \mathbb{N}. \quad (2.37)$$

The fermionic two-point correlations (we seek the ground state in the subspace with $N = 1$) read as

$$C_{ln} \equiv \langle c_l^+ c_n \rangle = \frac{1}{L} \sum_{k=1}^{L} e^{\frac{2\pi i (l-n)}{L} \theta \left(h - J \cos \left(\frac{2\pi k}{L}\right)\right)}, \quad (2.38)$$

where we indicated with $\theta$ the Heaviside step function $\theta(x) = (1 + \text{sgn}(x))/2$. The ambiguity in the definition of that function is reflected on the choice of the ground state, provided that condition \(2.37\) is satisfied\(^1\). In the presence of strong magnetic fields $|h| > 1$ all spins are aligned in the direction of the magnetic field

$$C_{ln}^{[h>1]} = \text{sgn}(h) \delta_{ln}. \quad (2.39)$$

In the absence of magnetic field, instead, the ground state is degenerate when the chain’s length is divisible by 4: for example, by choosing $\theta(0) \equiv \frac{1-\delta}{2}$, we get

$$C_{ln}^{[h=0]} = \begin{cases} \frac{\delta_{ln}}{2} - J \frac{(-1)^{\frac{n-l}{2}}}{L} \sin^{-1} \left(\frac{(n-l)\pi}{2L}\right) & l + n \text{ even} \quad L \equiv 0 \mod 4 \\ J \frac{(-1)^{\frac{n-l+1}{2}}}{L} \cot \left(\frac{(n-l)\pi}{2}\right) & l + n \text{ odd} \\ \frac{\delta_{ln}}{2} + J \frac{(-1)^{\frac{n-l+1}{2}}}{2L} \cos^{-1} \left(\frac{(n-l)\pi}{2L}\right) & l + n \text{ even} \quad L \equiv 1 \mod 4 \\ J \frac{(-1)^{\frac{n-l+1}{2}}}{2L} \sin^{-1} \left(\frac{(n-l)\pi}{2L}\right) & l + n \text{ odd} \end{cases} \quad L \equiv 2 \mod 4 \quad (2.40)$$

In general, for magnetic fields corresponding to non-degenerate ground states we have

$$C_{ln} = \left[ \frac{1}{2} + J \frac{1}{L} \frac{\sin \theta_j (n-l)}{\sin \frac{(n-l)\pi}{L}} \right] \delta_{ln} - (1 - \delta_{ln}) J \frac{\sin \theta_j (n-l)}{L} \frac{\sin \frac{(n-l)\pi}{L}}{\sin \frac{(n-l)\pi}{L}} \sin \frac{(n-l)\pi}{L}, \quad (2.41)$$

\(^1\)We stress that zero modes come always in pair, and the ground state cannot have a single excitation ($N = 1$). This condition is automatically fulfilled by the step function, which entails the presence or not of both excitations (depending on the value of $\theta(0) \in \{0, 1\}$)

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with the Fermi momentum defined as
\[ k_F = \frac{\pi}{L} \left( 2 \left\lceil \text{arccos} \left( \frac{h}{J} \right) + 1 \right\rceil - 1 \right). \] (2.42)

In the thermodynamic limit \( L \to \infty \) we find
\[ C \ln L \to \infty \quad \text{as} \quad k_F = \text{arccos} \left( \frac{h}{J} \right). \] (2.43)

Notice that the correlation matrix \( \Gamma \), defined in Eq. (2.34), becomes simpler when the number of JW fermions is conserved, as in the XX chain:
\[ \Gamma = (1 - 2J) \otimes \frac{1 + \sigma_y}{2} - (1 - 2C^T) \otimes \frac{1 - \sigma_y}{2} \sim (1 - 2C) \oplus (2C^T - 1). \] (2.44)

**Thermodynamic limit.** In the thermodynamic limit \( L \to \infty \) the momentum \( k_F \) becomes a continuum variable \( \phi \in (0, 2\pi] \), and the dispersion relation is as follows:
\[ \varepsilon(\phi) = \sqrt{(J \cos \phi - h)^2 + \gamma^2 \sin^2 \phi}. \] (2.45)

The critical models are characterized by the absence of a gap between the ground state and the first excited state, i.e., they correspond to the values of \( \gamma \) and \( h \) for which the following system of equations admits solution
\[ \begin{cases} J \cos(\phi) - h = 0 \\ \gamma \sin \phi = 0. \end{cases} \] (2.46)

There are two possibilities: \( \gamma = 0 \) and \( |h| < 1 \), and \( |h| = 1 \) for any value of \( \gamma \). The critical regions can be grouped in three classes, according to their physical properties [62]:

1. \( |h| = 1 \) and \( \gamma \neq 0 \): the dispersion relation is linear at low energies
\[ \varepsilon \sim |\gamma||\phi - \frac{1 - J}{2}\pi| \quad \phi \approx \frac{1 - J}{2}\pi \] (2.47)

and the critical behavior is described by a CFT of a free massless fermion in 1+1 dimension, with central charge \( c = \frac{1}{2} \);

2. \( |h| < 1 \) and \( \gamma = 0 \): in the low energy limit, the dispersion relation has two chiral modes
\[ \varepsilon \sim \sqrt{1 - h^2} |\phi - \varphi_\pm| \quad \varphi_\pm \approx \varphi_\pm = \pm \text{arccos} \left( \frac{h}{J} \right) \] (2.48)

and it is described by a CFT of a free massless boson in 1+1 dimension, with central charge \( c = 1 \);

1Here and in the rest of the work, \( \lceil x \rceil \) stands for the closest integer larger than \( x \) and \( \lfloor x \rfloor \) for the closest integer smaller than \( x \).
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3. \(|h| = 1\) and \(\gamma = 0\): the dispersion relation is quadratic at low energies

\[
\varepsilon \sim \frac{1}{2} \left( \varphi - \frac{1 + J}{2} - \pi \right)^2 \quad \varphi \approx \frac{1 + J}{2} + \pi ,
\]

hence the dynamical critical exponent \(z\) is equal to 2, and it can not be described by a CFT.

Furthermore, there is a special region, namely the circumference \(h^2 + \gamma^2 = 1\), in which the ground state is double degenerate and the subspace is the span of two completely separable states, \(i.e.\) states in which the entanglement entropies of any subsystem vanish. This is true exactly also for finite chains of even size, when \(J = 1\) [63].

Apart from these general considerations, any physical property of the system can be obtained from the correlations (2.34), which, in the thermodynamic limit, are given by

\[
f_n \equiv \langle a^+_l a^y_{l+n} \rangle = \delta_{n0} \quad g_n \equiv i \langle a^+_l a^y_{l+n} \rangle = \int_0^{2\pi} \frac{d\varphi}{2\pi} e^{i\varphi} J \cos \varphi + i\gamma J \sin \varphi - h .
\]

We stress once again that the correlations depend only on the distance between the Majorana fermions, because of translational invariance. In a system with one or more boundaries this is no longer true, however we will see in the next subsection that the boundaries just modify the structure of Eq. (2.50) preserving all other details.

2.1.2 Open boundary conditions

In this subsection we consider the XY model with open boundary conditions. Because of the boundaries, the Hamiltonian does not simplify in Fourier transform and, apart from specific cases, the diagonalization is more complicated. For this reason, we start considering the more general problem of diagonalizing a quadratic Hamiltonian. The standard method relies on the representation in terms of the Majorana fermions (2.33). The Majorana representation of the open XY chain reads as

\[
H_{XY}^{(OBC)} = \sum_{j,n=1}^{2L} (a^+_l a^y_{l+n}) \mathcal{H}_{jn} \left( \frac{a^x_n}{a^y_n} \right) \quad \text{with} \quad \mathcal{H}_{jn} = \begin{cases} \frac{iJ}{4} \gamma \sigma_x - i\sigma_y & n = l + 1 \\ \frac{b}{2} \sigma_y & n = l \\ \frac{b}{4} \gamma \sigma_x + i\sigma_y & n = l - 1 . \end{cases}
\]

In general, the block matrix \(\mathcal{H}\) is a purely imaginary skew-symmetric matrix, hence it can be block-diagonalized by an orthogonal transformation

\[
V_j \mathcal{H}_{jj'} V^T_{nj'} = \frac{1}{4} \delta_{jn} \delta_{l} \sigma_y \quad \sum_{j=1}^{2L} V_j V^T_{nj} = \delta_{jn} I .
\]

The parameters \(\varepsilon_l\) define the dispersion relation, and the fermions

\[
\begin{pmatrix} d_l^+ \\ d_l^- \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \sum_n V_{ln} \left( \frac{a^x_n}{a^y_n} \right) \quad H = \sum_{l=1}^{L} \varepsilon_l \left( d_l^- d_l^- - \frac{1}{2} \right) .
\]
diagonalize the Hamiltonian. Finally, the correlation matrix can be easily written in terms of $V$:

$$\Gamma_{nl} \equiv \left( \begin{array}{cc} a^x_n & a^y_n \\ a^y_n & a^x_n \end{array} \right) (\sigma^x_n \quad \sigma^y_n) - \delta_{ln} I = \sum_{j=1}^{L} V^T_{j} \sigma_j V_{jn}. \quad (2.54)$$

Up to now, we never used the particular form of the Hamiltonian, and Eqs. (2.52), (2.53), and (2.54) do hold for any quadratic Hamiltonian. Some simplifications occur considering the very form of the XY Hamiltonian with OBC (2.51). The matrix $H$, indeed, commutes with $\sigma^y \otimes E$, where $E_{ln} = \delta_{l+n} L_1$, hence the $H$'s eigenvectors can be chosen to be eigenstates of $\sigma^y \otimes E$. This means that the blocks $\tilde{\Phi}_n$ of the eigenvectors $\Phi$ have the general form

$$\tilde{\Phi}_n^\pm = \left( \begin{array}{c} \phi_n \\ \pm \phi_{L+1-n} \end{array} \right). \quad (2.55)$$

By substituting Eq. (2.55) into the eigenvalue equation we get

$$\begin{cases} \frac{J}{4} + \gamma \phi_{n+1} - \frac{h}{4} \phi_n = \frac{J}{4} - \frac{\gamma}{2} \phi_{n-1} = \pm \frac{\epsilon}{4} \phi_{L+1-n} & n = 2, \ldots, L - 1 \\ \frac{J}{4} + \frac{\gamma}{2} \phi_2 - \frac{h}{4} \phi_1 = \pm \frac{\epsilon}{4} \phi_L \\ - \frac{h}{4} \phi_{L-1} = \frac{J}{4} - \frac{\gamma}{2} \phi_L - \frac{\epsilon}{4} \phi_1. \end{cases} \quad (2.56)$$

From the system of equations above it is evident that $\phi_n$ is real for any $n$, and if $\epsilon/4$ is the eigenvalue corresponding to $\tilde{\Phi}^+$ then $-\epsilon/4$ is associated to the eigenvector $\tilde{\Phi}^-$. The normalization of the eigenvectors $\tilde{\Phi}^\pm$ implies

$$\sum_{l=1}^{L} \phi_l^{x_n} \phi_l^{x_{n'}} = \frac{1}{2} \delta_{kk'}, \quad \sum_{k} \phi_k^{x_n} \phi_k^{x_{n'}} = \frac{1}{2} \delta_{ln}, \quad (2.57)$$

hence the unitary matrix

$$U_{lk} = \left( \begin{array}{cc} \phi_l^{(x_k)} & \phi_l^{(x_k)} \\ i\phi_l^{(x_k)} & -i\phi_l^{(x_k)} \end{array} \right) \quad (2.58)$$

diagonalizes $H$ ($H U = U (\sigma_z \otimes D)$, with $D_{kk'} = \frac{\epsilon}{4} \delta_{kk'}$). The orthogonal matrix that block-diagonalizes the skew-symmetric Hermitian matrix can be obtained by multiplying $U$ to the right by the block diagonal matrix $e^{i \frac{\pi}{4} (1 - \sigma_z)} \otimes I$

$$V^T_{lk} = [U (e^{i \frac{\pi}{4} (1 - \sigma_z)} \otimes I)]_{lk} = \left( \begin{array}{cc} \phi_l^{(x_k)} & \phi_l^{(z_k)} \\ -s_k \phi_l^{(x_k)} & s_k \phi_l^{(z_k)} \end{array} \right), \quad (2.59)$$

where $s_k = \text{sgn}(\epsilon_k)$. Indeed, the auxiliary rotation transforms the diagonal blocks made of opposite eigenvalues (and hence proportional to $\sigma_z$) to skew-symmetric ones (i.e. proportional to $\sigma_y$)

$$e^{-i \frac{\pi}{4} (1 - \sigma_z)} \sigma_z e^{i \frac{\pi}{4} (1 - \sigma_z)} = \sigma_y. \quad (2.60)$$

---

1 This is no longer true adding a Dzyaloshinskii-Moriya-like interaction, e.g. $\sum_{l} \sigma^x_l \sigma^x_{l+1} = \sigma^y_l \sigma^y_{l+1}$. 

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Finally, the correlation matrix can be written as follows:

\[
\Gamma_{nl} = \sum_{\varepsilon_k} \left( \begin{array}{cc} \phi_{l\epsilon_k} & \phi_{l\epsilon_k} \\ -s_k \phi_{L+1-1\epsilon_k} & s_k \phi_{L+1-1\epsilon_k} \end{array} \right) \sigma_y \left( \begin{array}{cc} \phi_{n\epsilon_k} & -s_k \phi_{L+1-n\epsilon_k} \\ \phi_{n\epsilon_k} & s_k \phi_{L+1-n\epsilon_k} \end{array} \right) = 2i \left( \begin{array}{cc} 0 & s_k \phi_{l\epsilon_k} \phi_{L+1-n\epsilon_k} \\ s_k \phi_{n\epsilon_k} \phi_{L+1-l\epsilon_k} & 0 \end{array} \right). \tag{2.61} \]

Notice that the correlation functions corresponding to excited states which are Slater determinants (i.e. when a set of \(d\)-fermions is excited) can be obtained by reversing the signs \(s_k\) associated to the excited quasiparticles in Eq.(2.61). Indeed, such states are the ground states of the Hamiltonian in which the signs of the energies of the excited fermions have been reversed. This operation is equivalent to exchange the columns of the orthogonal matrix \(V\) associated to each excited fermion. In Chapter 5 we will discuss extensively the consequences of such transformation in order to analyze the excited states of the XY chain with periodic boundary conditions.

The system of equations (2.56) can be solved easily in the isotropic limit (XX model, \(\gamma = 0\)), and for \(\gamma = \pm 1\) (quantum Ising model). In the following paragraphs we focus on such systems.

**XX model.** The fermionic mapping (2.22) of the XX Hamiltonian (2.15) with OBC reads as

\[
H^{(OBC)}_{XX} = J \sum_{l=1}^{L-1} \left( c_{l+1}^\dagger c_l + c_{l+1}^\dagger c_l \right) - h \sum_{l=1}^{L} c_{l}^\dagger c_l + \frac{hL}{2}. \tag{2.62} \]

The number of JW fermions is conserved, indeed \(H = \sum_{l,n} c_{l}^\dagger H c_n\). The model can be solved by diagonalizing the tridiagonal symmetric Toeplitz matrix \(H\). The fermions that diagonalize \(H^{(OBC)}_{XX}\) are given by

\[
d_{k}^\dagger = \sqrt{\frac{2}{L+1}} \sum_{l=1}^{L} \sin \left( \frac{\pi kl}{L+1} \right) c_{l}^\dagger \quad \{d_{k}^\dagger, d_{p}^\dagger\} = \delta_{kp} \quad \{d_{k}, d_{p}\} = 0, \tag{2.63} \]

indeed, substituting (2.63) into the Hamiltonian (2.62) gives

\[
H^{(OBC)}_{XX} = \sum_{k=1}^{L} \left( J \cos \left( \frac{\pi k}{L+1} \right) - h \right) d_{k}^\dagger d_{k} + \frac{hL}{2}. \tag{2.64} \]

The ground state is not the vacuum of the operators \(d\), since all fermions with negative energy (inside the Fermi sea) are excited. This means

\[
\langle d_{k}^\dagger d_{k}\rangle = \delta_{kk} \theta \left( h - J \cos \left( \frac{\pi k}{L+1} \right) \right). \tag{2.65} \]

The fermionic two-point correlations can be obtained by expressing the operators \(c\) in terms of the \(d\)’s:

\[
C_{ln} = \langle c_{l}^\dagger c_{n}\rangle = \frac{2}{L+1} \sum_{k=1}^{L} \sin \left( \frac{\pi kl}{L+1} \right) \sin \left( \frac{\pi kn}{L+1} \right) \theta \left( h - J \cos \left( \frac{\pi k}{L+1} \right) \right). \tag{2.66} \]
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The ground state is degenerate whenever the argument of the Heaviside step function can vanish.

For strong magnetic fields $|h| > 1$

$$C_{ln}^{[h]>1} = \text{sgn}(h)\delta_{ln}$$ (2.67)

all spins are aligned in the direction of $h$, as in the periodic case (cf. (2.39)). On the other hand, in the absence of magnetic field, choosing for example $\theta(0) \equiv 1 - \frac{J}{2}$, we find

$$C_{ln}^{h=0} = \left\{ \begin{array}{ll}
\delta_{ln} + J(-1)^{\frac{l+n}{2}}(-1)^{\frac{l-n}{2}} \frac{l-n}{2(L+1)} & l + n \text{ even} \\
J(-1)^{\frac{l+n}{2}} \cot\left(\frac{(l+n)\pi}{2L+1}\right) + (-1)^{\frac{l-n}{2}} \cot\left(\frac{(l-n)\pi}{2L+1}\right) & l + n \text{ odd} \\
\delta_{ln} + J(-1)^{\frac{l+n}{2}} \sin^{-1}\left(\frac{(l+n)\pi}{2(L+1)}\right) + (-1)^{\frac{l-n}{2}} \sin^{-1}\left(\frac{(l-n)\pi}{2(L+1)}\right) & l + n \text{ even} \\
J(-1)^{\frac{l+n}{2}} \cot\left(\frac{(l+n)\pi}{2L+1}\right) + (-1)^{\frac{l-n}{2}} \cot\left(\frac{(l-n)\pi}{2L+1}\right) & l + n \text{ odd}
\end{array} \right. \quad (2.68)$$

In general, for magnetic fields corresponding to non-degenerate ground states we have

$$C_{ln} = \left[\frac{1}{2} + J\left(\frac{L}{2(L+1)} - \frac{k'_F}{\pi}\right)\right] \delta_{ln} - (1 - \delta_{ln}) \frac{J}{2(L+1)} \left[ \frac{\sin(k'_F(n-l))}{\sin\left(\frac{(n-l)\pi}{2L+1}\right)} \right] - \frac{\sin(k'_F(n+l))}{\sin\left(\frac{(n+l)\pi}{2L+1}\right)} \right]$$ (2.69)

with

$$k'_F = \pi\left(\frac{2\left[\arccos\frac{h}{2}\pi(L+1)\right] + 1}{2(L+1)}\right).$$ (2.70)

Observe that this definition does not coincide with the Fermi momentum $k_F$, namely $\pi N_F/L$, where $N_F$ is the number of fermions in the Fermi sea, indeed

$$k_F = \frac{\pi\left[\arccos\frac{h}{2}\pi(L+1)\right]}{L}. \quad (2.71)$$

Notice that the matrix of the two-point correlations is Toeplitz+Hankel in contrast with the Toeplitz matrix that arises considering periodic boundary conditions (cf. (2.40)). This has a very nice interpretation: the boundaries act as mirrors for the quantum correlations and, practically, the correlation functions in an open chain of length $L$ can be obtained by the correlation functions of the periodic chain of length $2(L+1)$, in which the open system is finally embedded (compare the correlations (2.40) with (2.68)). Indeed, Eq. (2.68) is sum of two terms, of the form of (2.40), that differ just for the exchange of $(l-n)$ for $(l+n)$, $(l+n)$ corresponding to the effective correlation between one fermion lying in the open chain and the “fermion image” reflected back by the boundary. We will describe in more details this mapping in Chapter 4, in which the corrections to the scaling of the entanglement entropies will be analyzed.

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1 A matrix $H$ is called Hankel matrix if $H_{ln} = H_{l+n}$, i.e. the elements of the anti-diagonals are equal.
2.1 XY model: the paradigm of “non-interacting” chains

Finally, in the thermodynamic limit \( L \to \infty \) the fermionic two-point correlations can be written as

\[
C_{ln} \xrightarrow{L \to \infty} \frac{1}{2} + J \left( \frac{1}{2} - \frac{k_F}{\pi} \right) \delta_{ln} - (1 - \delta_{ln}) J \left[ \frac{\sin(k_F(n-l))}{\pi(n-l)} - \frac{\sin(k_F'(n+l))}{\pi(n+l)} \right]
\]  

(2.72)

with \( k_F = \arccos(\frac{2}{L}) \). The unitary transformation \( d^\dagger \leftrightarrow d \), applied to any fermion in the Fermi sea, defines the excitations of the system, and results in the dispersion relation

\[
\varepsilon_k = \left| J \cos \left( \frac{\pi k}{L+1} \right) - h \right| \xrightarrow{L \to \infty} \varepsilon(\varphi) = |J \cos(\varphi) - h| \quad \varphi \in [0, \pi] .
\]  

(2.73)

Observe that the system is gapless for \( |h| < 1 \) and the dispersion relation is linear at low energies, however there is only one chiral mode. It is no accident that the number of chiral modes halves moving from periodic to open boundary conditions. In fact, associating the same central charge to each chiral mode, results in a halved effective central charge for open chains, i.e. the prescription of substituting \( c \) with \( \frac{c}{2} \) in the expressions relative to PBC. We will see that this substitution is indeed sufficient for characterizing the exponent of the correlation functions or the leading behavior of the entanglement entropies.

Ising model. The quantum Ising model with open boundary conditions is another special case that can be solved easily. It is given by the XY Hamiltonian (2.9) with \( \gamma = 1 \) (\( \gamma = -1 \) is completely equivalent to \( \gamma = 1 \), being the result of a rotation of \( \frac{\pi}{2} \) about the \( z \) axis), i.e. the Hamiltonian (2.22) with \( N = 0 \) and \( \gamma = 1 \)

\[
H_{\text{Ising}}^{(OBC)} = \frac{J}{2} \sum_{l=1}^{L-1} \left( c^\dagger_l c_{l+1} + c^\dagger_{l+1} c_l + H.c. \right) - h \sum_{l=1}^{L} c^\dagger_l c_l + \frac{hL}{2} .
\]  

(2.74)

The system of equations (2.56) can be written as

\[
\begin{align*}
J \phi_{n+1} - h \phi_n &= \varepsilon \phi_{L+1-n} \quad n = 1, \ldots, L-1 \\
-h \phi_L &= \varepsilon \phi_1 .
\end{align*}
\]  

(2.75)

The equations corresponding to \( n \) and \( L-n \) concern the same variables \( \phi_n, \phi_{n+1}, \phi_{L+1-n} \), and \( \phi_{L-n} \), hence it is convenient to consider them together. In particular we assume \( L \) even, but there are no complications in considering \( L \) odd

\[
\begin{align*}
J \phi_{n+1} &= h \phi_n + \varepsilon \phi_{L+1-n} \quad n = 1, \ldots, L/2 - 1 \\
h \phi_{L-n} + \varepsilon \phi_{n+1} &= J \phi_{L+1-n} \quad n = 1, \ldots, L/2 - 1 \\
J \phi_{n+1} - h \phi_L &= \varepsilon \phi_{L+1-n} \\
-h \phi_L &= \varepsilon \phi_1 .
\end{align*}
\]  

(2.76)

By defining \( \psi^\pm_n \equiv \phi_n + \frac{h}{2J\varepsilon} \phi_{L+1-n} \), with

\[
\cos \theta = \frac{h^2 - \varepsilon^2 - 1}{2J\varepsilon} ,
\]  

(2.77)
and by solving the (straightforward) recursion relation coming from the first two equations of the system (2.76), we get

\[
\begin{aligned}
\psi_n^\pm &= \left( \frac{h}{J + \epsilon e^{\pm i\theta}} \right)^{n-1} \psi_1^\pm \quad n = 1, \ldots, L/2 \\
\psi_L^+ &= e^{i\theta} \psi_L^- \\
\psi_1^+ &= \frac{J + \epsilon e^{-i\theta}}{J + \epsilon e^{i\theta}} \psi_1^-.
\end{aligned}
\]  

(2.78)

By comparing the first equation, with \( n = L/2 \), with the other two equations, we obtain the quantization condition

\[
\left( \frac{J + \epsilon e^{-i\theta}}{J + \epsilon e^{i\theta}} \right)^{L/2} = e^{i\theta}.
\]  

(2.79)

Actually, it is convenient to work with the variable \( k \), defined as

\[
e^{2ik} \equiv \frac{J + \epsilon e^{-i\theta}}{J + \epsilon e^{i\theta}} \Rightarrow \epsilon = -J \frac{\sin k}{\sin(k + \theta)}.
\]  

(2.80)

Eq (2.77) can be written as follows

\[
e^{ik} = \frac{h}{J + \epsilon e^{i\theta}} = \frac{J + \epsilon e^{-i\theta}}{h} e^{iLk} = e^{iLk}
\]  

(2.81)

and the system (2.76) becomes

\[
\begin{aligned}
\psi_n^\pm &= e^{\pm ik(n-1)} \psi_1^\pm \quad n = 1, \ldots, L/2 \\
\psi_L^+ &= e^{iLk} \psi_L^- \\
\psi_1^+ &= e^{-2ik} \psi_1^- \\
\psi_n^+ &= \phi_n + e^{\pm i(L+1)k} \phi_{L+1-n}
\end{aligned}
\]  

(2.82)

with the quantization conditions

\[
\epsilon_k = J \sqrt{1 + h^2 - 2Jh \cos k} \\
J \sin(Lk) = h \sin((L + 1)k).
\]  

(2.83)

By exploiting Eqs. (2.83), the original variables \( \phi_n \) can be written in the following equivalent forms

\[
\phi_n = N_k \sin((L + 1 - n)k) = \frac{N_k}{\epsilon_k} \left[ h \sin(nk) - J \sin((n - 1)k) \right]
\]  

(2.84)

where

\[
N_k^2 = \left( L - h \frac{J \cos k - h}{\epsilon_k^2} \right)^{-1}.
\]  

(2.85)

In fact Eqs. (2.83) and (2.84) are valid also for odd lengths \( L \). The pseudo-momenta \( k \) that solve the quantization conditions are real for \( |h| \geq \frac{L}{L+1} \), otherwise a complex pseudo-momentum \( k_0 \) appears. If \( hJ > 0 \) then \( k_0 \) is purely imaginary otherwise it has real part equal to \( \pi \). In the limit as \( |h| \) approaches \( \frac{L}{L+1} \) from the left, \( k_0 \) goes to 0 (or \( \pi \)) quadratically.
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\( h = \frac{L}{L+1} J \) the formula (2.84) is indeterminate for \( k_0 = 0 \) and we must take the derivative of (2.84) with respect to \( k \), obtaining

\[
\begin{align*}
\varepsilon_0 &= \frac{J}{L+1} \\
\phi_n^{(0)} &= \sqrt{\frac{3(1+L)}{L(1+2L)}} \left(1 - \frac{n}{L+1}\right)
\end{align*}
\]

(2.86)

\( k_0 \) defines the boundary bound state \( \hat{d}_{k_0}^\dagger |\emptyset\rangle \) which, in the thermodynamic limit, is degenerate with the ground state, up to terms exponentially small in the size of the chain. Indeed, the quantization conditions (2.83) for large \( L \) with the ground state, up to terms exponentially small in the size of the chain. In fact, for finite chains, the pseudo-momenta are different from \( \pi n \), for any integer \( n \ll L \), it is \( O(h^L) \). Finally, we get

\[
i \langle \hat{a}_i^\dagger \hat{a}_n^\dagger \rangle = \frac{J}{2L} \sum_{k} \frac{(e^{-iL} - h)(e^{i(l+k)k} - e^{i(l-n)k})}{\varepsilon_k - hJ \cos k - h \varepsilon_k},
\]

(2.91)

which has the same structure Toeplitz+Hankel observed in the XX chain (cf. (2.68)). In contrast to the XX chain, however, the symbol is not exactly the same as for periodic boundary conditions. In fact, for finite chains, the pseudo-momenta are different from \( \frac{2\pi n}{L} \), for any integer \( L \approx 2L \), and a new “effective” energy comes into play

\[
\varepsilon_{k_0}^{(L)} = \varepsilon_k - hJ \cos k - h \frac{L \varepsilon_k}{\varepsilon_k}.
\]

(2.92)
2. EXACTLY SOLVABLE SPIN CHAINS

As we are going to show, these differences disappear for large $L$. Indeed the quantization condition can be written as

$$\frac{L}{\pi} k - \frac{1}{\pi} \arctan \left( \frac{\sin(k)}{J - h \cos(k)} \right) \equiv n \in \{0, \ldots, L\}. \quad (2.93)$$

For $|h| \leq \sec(\frac{\pi}{2L})$ each pseudo-momentum is associated to a different $n$: for $Jh > 0$ $n = 0, \ldots L - 1$, otherwise $n = 1, \ldots L$; in particular $k_0$ corresponds to $n \in \{0, L\}$. On the other hand, for $|h| > \sec(\frac{\pi}{2L})$ there are two momenta associated to the same $n$. Once the integer $n$ becomes associated to two momenta, i.e. when $h = J \sec(\frac{\pi(2n+1)}{2L})$, one momentum corresponds to the special solution $k = \frac{\pi(2n+1)}{2L}$. This whole picture means that, for large $L$, the momenta $k$ are distributed almost uniformly in the interval $(0, \pi)$ and, in the thermodynamic limit, $k$ becomes a continuous variable and the sums can be turned into integrals with uniform measure (Euler-Maclaurin formula)

$$\frac{1}{L} \sum_k f_k \to \int_0^\pi \frac{dk}{\pi} f(k). \quad (2.94)$$

Finally, in the thermodynamic limit, the fermionic two-point correlations read as

$$i \langle a_x^\dagger a_y \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{Je^{-ik} - h(e^{i(l+n)k} - e^{i(l-n)k})}{\sqrt{1 + h^2 - 2h \cos k}} \quad (2.95)$$

and the connection with the corresponding periodic chain becomes evident (cf. Eq. 2.50 with $\gamma = 1$)

In the following section we go back over the question of entanglement, giving an overview of the basic techniques employed in the analysis of the entanglement entropies in systems that, like the XY model, have a free-fermion representation.

2.2 RDMs in “non-interacting” chains

The density matrix $\rho$ is defined as the positive semidefinite Hermitian operator whose product with any observable has trace equal to the expectation value of the observable

$$\langle \hat{O} \rangle = \text{Tr} \rho \hat{O}. \quad (2.96)$$

In particular, if the system is a spin-$s$ lattice, i.e. in each lattice site the physical degrees of freedom represent $SU(2s + 1)$, the density matrix has a natural expansion in terms of the generators of $SU(2s + 1)$. The generators $T^\alpha$ are represented by traceless Hermitian matrices that, in the fundamental representation, satisfy

$$T^\alpha T^\beta = \frac{\delta_{\alpha\beta}}{4s + 2} + \frac{1}{2} \sum_{\gamma=1}^{4s(s+1)} (i f_{\alpha\beta\gamma} + d_{\alpha\beta\gamma}) T^\gamma \quad \text{Tr} T^\rho = 0, \quad (2.97)$$
2.2 RDMs in “non-interacting” chains

where the \( f \)'s are the structure constants, antisymmetric in all indices, whilst the \( d \)'s are symmetric. Any operator of the theory can be represented in the basis of the generators

\[
\bigotimes_{l \in S \subset \Omega} T^{\alpha_l}_l,
\]

(2.98)

where \( \Omega \) is the set of lattice sites. In fact the density matrix has the following representation

\[
\rho_{\Omega} = \frac{1}{(2s + 1)^{2L}} \sum_{S \subset \Omega} \sum_{\alpha_l = 1}^{2s+1} (4s + 2)^{|S|} \langle \bigotimes_{l \in S} T^{\alpha_l}_l \rangle \bigotimes_{l \in S} T^{\alpha_l}_l,
\]

(2.99)

as one can verify considering the trace with any operator, by using that the product of two different generators is traceless (cf. (2.97)). In particular, the density matrix of a spin-\( \frac{1}{2} \) chain can be written as

\[
\rho_{\Omega} = \frac{1}{2^{2L}} \sum_{S \subset \Omega} \langle \prod_{l \in S} \sigma^{\alpha_l}_l \rangle \prod_{l \in S} \sigma^{\alpha_l}_l.
\]

(2.100)

Actually, we never used that \( \Omega \) consists of all sites, hence \( \rho_{\Omega} \) can describe both the full lattice and a part of it. Eq. (2.99), and in particular Eq. (2.100), is what we call “spin representation” of the density matrix, since \( \Omega \) is a set of sites occupied by spins. And \( \rho_{\Omega} \) is the reduced density matrix of the subsystem specified by \( \Omega \). The representations above are the quantitative version of the claim that the reduce density matrix is “sum of all correlations”, but it is not particularly useful in practice, since the sum extends over the full subspace.

We now consider the fermionic mapping of a spin-\( \frac{1}{2} \) chain by means of the Jordan-Wigner transformation. By retracing the same steps that have led to Eq. (2.99), the density matrix of the total system can be easily written in terms of the Majorana fermions \( a_l, a^\dagger_l \)

\[
\rho = \frac{1}{2^L} \sum_{S \subset \{1, \ldots, 2L\}} \langle \prod_{l \in S} a_l \rangle \prod_{l \in S} a_l,
\]

(2.101)

where \( L \) is the chain’s length, the symbols \(< \) and \(> \) indicate that the two products have reversed ordering, and we defined \( a_{2l-1} \equiv a^\dagger_l \) and \( a_{2l} \equiv a^\dagger_l \). In contrast to the spin representation, in which the indices of the generators correspond exactly to the physical position, the indices of the Majorana fermions in the fermionic representation (2.101) have not a very physical meaning. Indeed the JW fermions have an intrinsic non-local nature (cf. (2.19)) and it is not obvious how to integrate over a part of the space. The density matrix obtained by summing over all subsets of a set \( \Omega \subset \{1, \ldots, 2L\} \) (for a better analogy with the spin representation, \( 2l \in \Omega \) iff \( 2l - 1 \in \Omega \)) is usually called the reduced density matrix in the fermionic representation

\[
\rho^{inf}_{\Omega} = \frac{1}{2^L} \sum_{S \subset \Omega} \langle \prod_{l \in S} a_l \rangle \prod_{l \in S} a_l.
\]

(2.102)

The fermionic reduced density matrix does depend on the representation: it can not have a direct physical meaning. Nevertheless, the fermionic representation is extremely useful when the
Jordan-Wigner transformation maps the Hamiltonian of spins into a quadratic Hamiltonian of fermions. In fact, the Wick theorem is equivalent to the fact that the fermionic reduced density matrix is Gaussian, i.e. it can be written as the exponential of a quadratic form

$$\rho_{\Omega}^{fer} = \frac{1}{Z[W]} e^{\sum_{i,n} a_i^\dagger a_i a_n^\dagger a_n},$$

(2.103)

where the constant $Z[W]$ ensures the normalization. The spectrum of the density matrix can be obtained by diagonalizing the matrix $W$, which has dimension $2\ell \times 2\ell$, whilst the subspace has dimension $2\ell$, where $\ell = |\Omega|/2$. Indeed, the orthogonal transformation that block-diagonalizes $W$ defines a set of fermions $d$ that diagonalize the quadratic operator in the exponent (cf. Eqs. (2.52) and (2.53))

$$\rho_{\Omega}^{fer} \equiv 1_{Z[W]} e^{\sum_k \omega_k (d_k^\dagger d_k - \frac{1}{2})} = \prod_k \frac{e^{-\frac{\omega_k}{2}} + 2 \sinh(\frac{\omega_k}{2}) d_k^\dagger d_k}{2 \cosh(\frac{\omega_k}{2})},$$

(2.104)

where $\omega_k$ are the eigenvalues of $W$. The eigenvalues and eigenvectors of $\rho_{\Omega}^{fer}$ are given by

$$|S\rangle \equiv \prod_{k \in S} d_k^\dagger |\emptyset\rangle \quad \lambda_S = \frac{\prod_{k \in S} e^{\omega_k}}{\prod_k (1 + e^{\omega_k})}.\quad (2.105)$$

The matrix $W$ is in direct relation with the correlation matrix $\Gamma_{ij} \equiv \langle a_j a_i \rangle - \delta_{ij}$: from Eq. (2.104) it follows that

$$\langle d_k^\dagger d_{k'} \rangle = \delta_{kk'} (1 + e^{-\frac{\omega_k}{2}})^{-1} \quad \langle d_k d_{k'} \rangle = 0,$$

(2.106)

hence $\Gamma$ can be obtained from Eq. (2.53) at once

$$\Gamma = \tanh \frac{W}{2}.\quad (2.107)$$

Finally, the eigenvalues of the density matrix in the fermionic representation can be expressed in terms of the eigenvalues $\nu_i$ of the correlation matrix as follows

$$\lambda_S = \prod_i \left(\frac{1 + \sigma_i \nu_i}{2}\right) \quad \text{where} \quad \sigma_i = \begin{cases} 1 & k \in S \\ -1 & \text{otherwise}. \end{cases} (2.108)$$

Notice that $\Gamma$ is a purely imaginary skew-symmetric matrix, hence the eigenvalues come in pairs of opposite sign ($\nu$, $-\nu$). The product in (2.108) runs over the pairs of eigenvalues. Eqs. (2.105) and (2.108) are a clear manifestation of the symmetries characterizing non-interacting fermion systems.

In conclusion, if a fermionic representation exists in which the physical reduced density matrix (2.100) is equal to a Gaussian fermionic density matrix (2.103) then not only the entanglement entropies but the entire spectrum can be obtained by diagonalizing the correlation matrix. This means that we can solve a problem with $2\ell$ degrees of freedom by diagonalizing a skew-symmetric matrix $2\ell \times 2\ell$, which requires a computational effort growing as $\ell^3$. But this is
not the end of the story. In the last section we have seen that the correlation matrix in the XY model is a structured matrix (block Toeplitz for PBC, and block Toeplitz+Hankel for OBC), hence the computational complexity can be further reduced and the entanglement entropies can be even worked out analytically. In the section below we discuss the relation between spin and fermionic representation. After that, we review the techniques and the basic analytical results obtained for the entanglement entropies in the XY model.

2.2.1 Spin representation vs fermionic representation

The fermionic representation of the RDM relies on the JW transformation

$$a_i^{x,y} = (\prod_{j < l} \sigma_j^x) \sigma_l^{x,y} a_{l-1}^{x,y} \sigma_{l-1}^x. \quad (2.109)$$

The string of $\sigma_z$, which we called $a_z$, makes the transformation non local: once fixed the set $\Omega$ (characterizing the subsystem in the spin representation), Eq. (2.100) turns out to be different from Eq. (2.102). In order to see such differences we rewrite (2.100) in terms of the Majorana fermions

$$\rho_\Omega = \frac{1}{2^{2N}} \sum_{S \subseteq \Omega} \sum_{a_{l-1}^{x,y}, a_{l}^{o,x}} \langle \prod_{l \in S} (a_{l-1}^{z,0} a_{l}^{0}) \prod_{l \in S} (a_{l-1}^{x}, a_{l}^{o}) \rangle. \quad (2.110)$$

$a_l^z$ commutes with $a_{l}^{o}$ and with $a_j^{x,y}$ for any $j > l$ but it anticommutes with $a_j^{x,y}$ for any $j \leq l$

$$a_l^z a_{l}^{o} = s_l^{o} a_{l}^{o} a_l^z \quad \text{with} \quad s_l^{o} = \begin{cases} 1 & \alpha = z \land l < 0 \\ -1 & \text{otherwise} \end{cases}. \quad (2.111)$$

hence the strings in Eq. (2.110) can be moved to the right (or to the left) freely: the signs coming from the expectation values simplify with those from the operators

$$\rho_\Omega = \frac{1}{2^{2N}} \sum_{S \subseteq \Omega} \sum_{a_{l-1}^{x,y}, a_{l}^{o,x}} \langle \prod_{l \in S} \sigma_l^{z} \prod_{l \in S} a_{l}^{z} \prod_{l \in S} a_{l}^{o} \prod_{l \in S} (a_{l-1}^{z,0} a_{l}^{0}) \rangle. \quad (2.112)$$

The factor

$$\langle \prod_{l \in S \cup Z} \sigma_l^{z} \prod_{l \in S} a_{l}^{z} \rangle \quad (2.113)$$

consists of $\sigma_z$’s that can be in $S$, $\Omega \setminus S$, but also outside of $\Omega$. The $\sigma_z$’s in $S$ are irrelevant because they can be reabsorbed into the sum over all possible configurations of $a_j^{x,y}$, indeed $\sigma_l^{z} a_{l}^{x,y} = \pm i a_{l}^{y,x}$, however they are responsible for a minus sign, due to the factor $1$. Thus we get

$$\rho_\Omega = \frac{1}{2^{2N}} \sum_{S \subseteq \Omega} (-1)^{|S|} \langle \prod_{l \in Z} \sigma_l^{z} \prod_{l \in S} a_{l}^{z} \sum_{a_{l-1}^{x,y}} \langle \prod_{l \in Z} \sigma_l^{z} \prod_{l \in S} a_{l}^{z} \prod_{l \in S} a_{l}^{0} \prod_{l \in S} (a_{l-1}^{z,0} a_{l}^{0}) \rangle. \quad (2.114)$$

Analogously, the $\sigma_z$’s in $Z$ in the expression $\prod_{l \in S} a_{l}^{z}$ can be neglected because they result essentially on a reordering of the sets $Z$. The number of $\sigma_l^{z}$, where $l \in S$, is equal to the

\footnote{One $i$ comes from the expectation value and one from the corresponding operator.}
number of sites that belong to $S$ and are greater than or equal to $\tilde{l}$. Thus the number of all $\sigma_z \in S$ is equal to $\frac{|S|(|S|+1)}{2}$. We can take into account the $\sigma_z$’s outside $\Omega$ by defining the region $\tilde{\Omega}$ such that $\Omega \cap \tilde{\Omega} = \emptyset$ and

$$\prod_{l \in S} a_l^\dagger = \prod_{l \in \Omega \cap \tilde{\Omega} \subset \Omega} \sigma_l^\dagger \prod_{l \in S \setminus \Omega} \sigma_l^\dagger. \quad (2.115)$$

Finally we get

$$\rho \equiv \frac{1}{2^{|S|}} \sum_{\substack{S,Z \in \Omega \setminus \tilde{\Omega} \subset \tilde{\Omega}}} (-1)^{|S|(|S|-1)} \prod_{l \in \tilde{\Omega}} \sigma_l^\dagger \prod_{l \in S \setminus \tilde{\Omega}} \sigma_l^\dagger \prod_{l \in S \setminus \Omega} (\prod_{l \in Z} \sigma_l^\dagger \prod_{l \in S \setminus Z} \sigma_l^\dagger)^{\alpha_l^\dagger \alpha_l}, \quad (2.116)$$

that is to say

$$\rho \equiv \frac{1}{2^{|S|}} \sum_{\substack{S,Z \in \Omega \setminus \tilde{\Omega} \subset \tilde{\Omega}}} \left[ \prod_{l \in \tilde{\Omega}} \sigma_l^\dagger \prod_{l \in S \setminus \tilde{\Omega}} \sigma_l^\dagger \prod_{l \in S \setminus \Omega} (\prod_{l \in Z} \sigma_l^\dagger \prod_{l \in S \setminus Z} \sigma_l^\dagger)^{\alpha_l^\dagger \alpha_l} \right] \prod_{l \in S \setminus \Omega} (\alpha_l^\dagger a_l^\dagger) . \quad (2.117)$$

This expression is exactly equal to (2.102) if $\tilde{\Omega}_S = \emptyset$, for any $S$. In fact, this means that the subsystem must be connected. The reason why holes are forbidden is that, if the subsystem is disjoint, we could consider the subset $S$ describing an odd number of fermions to the left and to the right of the hole. And the string of $\sigma_z$ belonging to the hole would appear in $\prod_{l \in S} a_l^\dagger$ (cf. Eq. (2.115)), resulting in $\tilde{\Omega}_S \neq \emptyset$.

In conclusion, we proved the fundamental result: the reduced density matrix of a spin block in a model with a free-fermion representation is Gaussian: the spectrum and the eigenvectors can be constructed by diagonalizing the correlation matrix. In the next section we exploit this mapping for computing the entanglement entropies in the XY model.

An interesting question is whether or not a fermionic mapping (perhaps different from the JW one (2.109), discussed in Ref. [29]) exists such that the RDM of a disjoint subsystem in a “non-interacting” model can be put in the form (2.103). We consider the subsystem that consists of two spins at the distance of two lattice spacing in an open XX chain of 4 spins in absence of magnetic field. This is probably the simplest example of disjoint subsystem in a chain that can be mapped into free fermions, however it is sufficient to disprove the existence of a mapping into a Gaussian RDM of fermions. The RDM is given by

$$\rho = \frac{1}{4} \left[ \sigma_1^z \sigma_3^z \sigma_1^x \sigma_3^x + \langle \sigma_1^y \sigma_3^y \rangle \sigma_1^y \sigma_3^y + \langle \sigma_1^y \sigma_3^x \rangle \sigma_1^y \sigma_3^x + \langle \sigma_1^x \sigma_3^y \rangle \sigma_1^x \sigma_3^y + \langle \sigma_1^x \sigma_3^x \rangle \sigma_1^x \sigma_3^x + I \right] \quad (2.118)$$

but the expectation values of products of $\sigma_z$ vanish because of the symmetries of the problem, and we get

$$\rho = \frac{1}{4} I + \frac{1}{10} a_2^y a_2^y a_4^y a_4^y + \frac{1}{10} a_4^x a_2^x a_4^x a_2^x . \quad (2.119)$$

Because $\rho$ commutes with $\sigma_2^z$ we can write

$$\rho = \frac{1 + \sigma_2^z}{2} \rho_+ + \frac{1 - \sigma_2^z}{2} \rho_-, \quad (2.120)$$

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2.2 RDMs in “non-interacting” chains

The density matrices \( \rho_{\pm} \) are fermionic density matrices restricted to the space of the first and the third fermion. However, they are not Gaussian, indeed the Wick theorem does not hold:

\[
\text{Tr}[\rho_{\pm} c_1^\dagger c_3] = 0 \quad \text{and} \quad \text{Tr}[\rho_{\pm} c_1^\dagger c_1] \text{Tr}[\rho_{\pm} c_3^\dagger c_3] - \text{Tr}[\rho_{\pm} c_1^\dagger c_3] \text{Tr}[\rho_{\pm} c_3^\dagger c_1] = -\frac{1}{25}.
\]

Anyway, they are quadratic operators and are diagonalized by the fermions

\[
\rho_{\pm} = \frac{1}{4} I \pm \frac{d_+^\dagger d_+ - d_-^\dagger d_-}{5},
\]

hence the spectrum of \( \rho \), which is equal to the spectrum of \( \rho_{\pm} \), is given by

\[
\lambda_l = \frac{1}{20} + \frac{1}{4} \left( \frac{l}{4} \right) \left( \frac{9}{20} \right).
\]

If a fermionic mapping that makes the density matrix Gaussian would exist, then its eigenvalues should be of the form (cf. (2.108))

\[
\lambda_l^{(Gauss)} = \frac{1}{2} + (-1)^{l+1} \nu_1 - (-1)^l \nu_2
\]

and \( \nu_{1,2} \) could be chosen as

\[
\nu_1 = \lambda_4 - \lambda_2 + \lambda_3 - \lambda_1 = \frac{2}{5}
\]

\[
\nu_2 = \lambda_4 - \lambda_3 + \lambda_2 - \lambda_1 = \frac{2}{5}.
\]

In fact the conditions (2.126) do not give the correct answer

\[
\lambda_l^{(Gauss)} = \frac{9}{100} \left( \frac{21}{100} \right) \left( \frac{21}{100} \right) \left( \frac{49}{100} \right).
\]

This example is evidence of the difficulties in obtaining the spectrum of the RDM associated to a disjoint subsystem: *the excitations that diagonalize the RDM do not behave as free fermions!* In chapter 3 we will describe a method to deal with such objects.

### 2.2.2 Entanglement entropies of a spin block in the XY model

In this subsection we consider the entanglement entropies of a spin block of length \( \ell \). From Eq. (2.108) it follows that the Reny entropies can be written as

\[
S_\alpha = \frac{\log \text{Tr}\rho_\alpha}{1 - \alpha} = \frac{1}{1 - \alpha} \sum_{l=1}^\ell \log \left[ \left( \frac{1 + \nu_l}{2} \right)^\alpha + \left( \frac{1 - \nu_l}{2} \right)^\alpha \right],
\]

while the entanglement entropy reads as

\[
S_{v.N.} = \lim_{\alpha \to 1^+} S_\alpha = -\sum_{l=1}^\ell \left( \frac{1 + \nu_l}{2} \log \frac{1 + \nu_l}{2} + \frac{1 - \nu_l}{2} \log \frac{1 - \nu_l}{2} \right).
\]
2. EXACTLY SOLVABLE SPIN CHAINS

Here we follow the method introduced by Jin and Korepin in [23] to calculate analytically the entanglement entropies of a block in the XY chain. The sum over the eigenvalues of the correlation matrix $\lambda$ can be recast as the integral in the complex plane of a function, with poles at $\nu_i$, over a closed path that encircles the poles. Indeed we have

$$S_\alpha = \lim_{\epsilon \to 0^+} \frac{1}{4\pi i} \sum_{l=1}^{2\ell} \oint_{C_\epsilon} e_\alpha(1 + 2\epsilon, \lambda) \frac{d\lambda}{\lambda - \nu_l} = \lim_{\epsilon \to 0^+} \frac{1}{4\pi i} \sum_{l=1}^{2\ell} e_\alpha(1 + 2\epsilon, \lambda) d\log \prod_{l=1}^{2\ell} (\lambda - \nu_l),$$  (2.130)

where

$$e_\alpha(x, y) \equiv \begin{cases} \frac{-x+y}{2} \log \frac{x+y}{2} - \frac{x-y}{2} \log \frac{x+y}{2} & \alpha = 1 \\ \frac{1}{1-\alpha} \log \left[ \left( \frac{x+y}{2} \right)^\alpha + \left( \frac{x-y}{2} \right)^\alpha \right] & \alpha > 1, \end{cases}$$  (2.131)

and $C_\epsilon$ encircles the interval $[-1, 1]$ at the distance $\epsilon$. The shift of $2\epsilon$ in the argument of $e_\alpha$ is used for avoiding the logarithmic cuts of $e_\alpha$.

The matrix $\lambda I - \Gamma$ has the same structure of the matrix $\Gamma$, i.e. it is block Toeplitz for periodic boundary conditions and block Toeplitz+Hankel for open boundary conditions. The logarithm of the determinant of $\lambda I - \Gamma$ can be worked out by using the known results on the behavior of the determinants of asymptotically large block Toeplitz matrices. The analytic expression of the entanglement entropies in the XY chain with periodic boundary conditions has been obtained for example in [65], but the simpler result relative to the XX chain came before [23], since the block Toeplitz matrix turns out to be a Kronecker product between a Toeplitz matrix and the constant $2 \times 2$ matrix $\sigma_y$. On the other hand, the analogous results for open boundary conditions have not been obtained for any value of the anisotropy constant $\gamma$ and magnetic field $h$. Up to now, only the entanglement entropies of the open XX chain have been computed analytically [11]. In the chapter 4 we will analyze in detail the Rényi entropies and the entanglement entropy of the XX chain both with periodic and open boundary conditions. Now, we just report the results obtained in [66] for the entanglement entropy in the limit of infinite subsystem $\ell \to \infty$ in the XY chain with PBC.

The idea is to substitute the asymptotic expansion of the determinant into Eq. (2.132). This operation is tricky, because we are commuting the limit of large lengths $\ell$, with the limit appearing in Eq. (2.132). By checking the analytical results against numerics, it follows that the two limits indeed commute. Finally, the entanglement entropy in the XY model with PBC is given by [66]

$$S_{v,N} = \begin{cases} \frac{1}{6} \left[ \log \left( \frac{k^2}{\sqrt{1-k^2}} \right) + (1 - k^2) \frac{4I(k)I(\sqrt{1-k^2})}{\pi} \right] + \log 2 & h < 1 \\ \frac{1}{12} \left[ \log \left( \frac{k^2}{\sqrt{1-k^2}} \right) + (2k^2 - 1) \frac{4I(k)I(\sqrt{1-k^2})}{\pi} \right] & h > 1 \end{cases}$$  (2.133)

where $I(x)$ is the complete elliptic integral of the first kind

$$I(x) = \int_0^1 \frac{dz}{\sqrt{(1-z^2)(1-x^2 z^2)}},$$  (2.134)
and

\[
k = \begin{cases} 
\frac{\sqrt{h^2 + \gamma^2 - 1}}{\gamma} & \sqrt{1 - \gamma^2} < h < 1 \\
\frac{\sqrt{1 - h^2 - \gamma^2}}{\sqrt{1 - h^2}} & 0 < h < \sqrt{1 - \gamma^2} \\
\frac{\gamma}{\sqrt{h^2 + \gamma^2 - 1}} & h > 1.
\end{cases}
\] (2.135)

Notice that the entanglement entropy diverges as \(\gamma\) and \(h\) approach critical values (we are considering infinite blocks). In Chapter 4 we will verify that the entanglement entropy in the XX chain with \(h < 1\) diverges as the logarithm of the block’s length with the prefactor \(\frac{1}{3}\), according to the CFT prediction (1.57) with central charge \(c = 1\).
2. EXACTLY SOLVABLE SPIN CHAINS
3. Entanglement entropies of disjoint subsystems

The asymptotic behavior of the quantities determining the Rényi entropies of an interval $A$, of length $\ell$, in an infinite one-dimensional critical system whose scaling limit is described by a CFT, is given by (cf. \(1.33\), \(1.56\))

$$\text{Tr} \rho_A^\alpha \simeq c_\alpha \left( \frac{\ell}{a} \right)^{c_\alpha \frac{c_1}{6} \left( \alpha - \frac{1}{\alpha} \right)} F_\alpha(x),$$

where $c$ is the central charge of the underlying CFT and $a$ is the lattice spacing. Thus the Rényi entropies (and in particular the von Neumann one for $\alpha = 1$) give one of the best ways of detecting the value of the central charge.

The entanglement entropy of two disjoint intervals in a CFT (and also in massive theories) has attracted attention only recently, when it has been recognized that it is sensitive to universal details of the CFT that are not encoded in the central charge. In fact it is connected with the full spectrum of operators of the CFT underlying the lattice model \([142628]\).

We consider here the case of two disjoint intervals $A = A_1 \cup A_2 = [u_1, v_1] \cup [u_2, v_2]$ depicted in Fig. 3.1. By global conformal invariance, in the thermodynamic limit, $\text{Tr} \rho_A^\alpha$ can be written as

$$\text{Tr} \rho_A^\alpha = c_\alpha^2 \left( \frac{u_1 - v_1}{|u_1 - v_1|} \frac{u_2 - v_2}{|u_2 - v_2|} \right)^{\frac{1}{\alpha}} F_\alpha(x),$$

where $x$ is the four-point ratio

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

Normalizing such that $F_\alpha(0) = 1$, $c_\alpha$ turns out to be the same non-universal constant appearing in Eq. (3.1). The universal function $F_\alpha(x)$ depends explicitly on the full operator content of the theory and must be calculated case by case. It is not equal to 1 identically because the $n$-sheeted Riemann surface $\mathbb{R}_n[A]$, where the fields of the path integral giving $\text{Tr} \rho^\alpha$ are defined, can not be uniformised to the complex plane when $A$ consists of disjoint blocks \([1426]\), as instead it happens for a single interval (see Sec. 1.2.1).
3. ENTANGLEMENT ENTROPIES OF DISJOINT SUBSYSTEMS

**Figure 3.1:** $\hat{S}_\alpha$ vs. $S_\alpha$ - Typical bipartition: the subset $A$ is the union of two disjoint intervals $A_1$ and $A_2$ of length $\ell_1$ and $\ell_2$ respectively. The block of length $r$ separating them is denoted by $B_1$. The ‘environment’ is $B = B_1 \cup B_2$. The thermodynamic limit is obtained by sending the total length $L \to \infty$, while $\ell_1, \ell_2, r$ remain finite (i.e. the length of $B_2$ goes to $\infty$).

The symmetry that makes the Rényi entropies of a subsystem equal to those relative to the rest of the system (prepared in a pure state) is manifested (in the thermodynamic limit) in the parity-symmetry about $x = \frac{1}{2}$ of $F_\alpha(x)$.

In fact, up to now, the universal function $F_\alpha(x)$ has been determined only for a free boson compactified on a circle [14], which corresponds to the critical XXZ Heisenberg chain (to give an example of a lattice model) as well as to the Luttinger liquid, and recently for the Ising universality class [27]. In both cases only the result for integer $\alpha > 1$ has been obtained. The analytic continuation to real $\alpha$ for general $x$ (in order to get the entanglement entropy) is still an open problem: only the behavior in some limits is analytically known. Notice, moreover, that the CFT calculations are quite complicated, and the numerical checks have proved to be a very important support to the theoretical predictions. The first attempt to check the CFT results was in Ref. [28], where the entanglement entropies of the XXZ chain have been obtained by means of exact diagonalization techniques. Unfortunately, the numerical results are limited to relatively small system sizes (at most 30 spins) and only few general properties (like the dependence on the Luttinger parameter) have been checked: large oscillating corrections to the scaling have made impossible a quantitative comparison for $F_\alpha(x)$. These problems have been partially overcome attacking the problem by approximate methods, as in Ref. [67], where the authors used a tree tensor network (TTN) algorithm for the quantum Ising model, as well as MonteCarlo simulations of the corresponding classical 2D one. It is notable that approximate techniques have been employed for the quantum Ising model, which does have a free-fermion representation. This is because, as emphasized at the end of the previous chapter,
3.1 RDM of disjoint blocks in XY chains

We start the analysis of the entanglement of disjoint subsystems from the Majorana representation (2.117) of the RDM associated to the subsystem corresponding to the sites belonging to the set \( \Omega \):

\[
\rho_{\Omega} = \frac{1}{2^{n_{\Omega} + n_{\bar{\Omega}}}} \sum_{s, z \in \Omega \cup \bar{\Omega}, n_{\Omega}, n_{\bar{\Omega}} \geq 0} \left[ \prod_{l \in \Omega} \sigma_l^i \right] \sum_{a^z_l \in \bar{\Omega}} \left[ \prod_{l \in \bar{\Omega}} \sigma_l^i \right] \prod_{l \in Z} (a^z_l a^z_l)^{n_{\bar{\Omega}}} \prod_{l \in Z} (a^z_l a^z_l)^{n_{\bar{\Omega}}}.
\]  

(3.4)

Remind \( a_{2l-1} = a^z_l = c_l + c_l^\dagger \) and \( a_{2l} = a^z_l = i(c_l - c_l^\dagger) \) are Majorana fermions, where \( c_l \) are the Jordan Wigner fermions (cf. Eq. (2.19)). \( a^z_l \) is the string \( \prod_{j \leq l} \sigma_j^z \) and \( \bar{\Omega}_S (\Omega \cap \bar{\Omega} = \emptyset) \) is defined by

\[
\prod_{l \in S} a^z_l = \prod_{l \in \bar{\Omega}_2 \cap \Omega} \sigma_l^z \prod_{l \in \bar{\Omega}_S \cap \bar{\Omega}} \sigma_l^z.
\]  

(3.5)

We consider a subsystem made of two disjoint blocks \( A_1 \) and \( A_2 \) (in the following we assume that the first site of the chain is the first site of \( A_1 \)). Eq. (3.4) can be simplified a little, indeed \( \bar{\Omega}_S \) is different from \( \emptyset \) iff the set \( S = S_1 \cup S_2 \) (\( S_1 \subset A_1 \), \( S_2 \subset A_2 \)) has an odd number of sites in \( A_2 \) (i.e. \(|S_2|\) is odd), in which case it is equal to the product \( a^z_{B_1} \equiv \prod_{l \in B_1} \sigma_l^z \) of the \( \sigma_z \)'s lying in the intermediate region \( B_1 \) between \( A_1 \) and \( A_2 \) (see Fig. 3.1). Incidentally, as long as the Hamiltonian conserves the parity of the number of fermions (and the symmetry is not broken as instead it happens e.g. in the ordered phase of the Ising model, cf. (2.89)), the expectation value of an odd number of fermions vanishes. This means that \(|S_1|\) has the same parity of \(|S_2|\).

In fact Eq. (3.4) can be rewritten as

\[
\rho_{A_1 \cup A_2} = \frac{1}{2^{n_1 + n_2}} \left[ \sum_{\text{even}} \langle O_1 O_2 \rangle O_2^1 O_1^1 + \sum_{\text{odd}} \langle O_1 a^z_{B_1} O_2 \rangle O_2^1 a^z_{B_1} O_1^1 \right],
\]  

(3.6)

where the two sums are intended over all possible products of Majorana fermions belonging to each interval and even/odd refers to the parity of the number of Majorana operators in the block \( A_2 \) (and \( A_1 \), if the parity is conserved). We introduced the ‘short’ \( O_{1,2} \) for a general product of Majorana operators belonging to \( A_{1,2} \).

These observations open the way for a generalization of Eq. (2.120), which we obtained in the special case of two spins at the distance of two lattice spacing in the open XX chain of 4 spins. Indeed the string \( a^z_{B_1} \) (which has eigenvalues \( \pm 1 \)) commutes with the reduced density matrix. Thus we can write

\[
\rho_{A_1 \cup A_2} = \frac{1 + a^z_{B_1}}{2} \rho_{A_1 \cup A_2} + \frac{1 - a^z_{B_1}}{2} \rho_{A_1 \cup A_2},
\]  

(3.7)

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with $\rho_{A_1 \cup A_2}^\pm$ the fermionic density matrices

$$\rho_{A_1 \cup A_2}^\pm = \frac{1}{2^{\sigma_A + 2}} \left[ \sum_{\text{even}} \langle O_1 O_2 \rangle O_1^\dagger O_2^\dagger \pm \sum_{\text{odd}} \langle O_1 a_{A_1}^\dagger O_2 \rangle O_1^\dagger O_2^\dagger \right]. \quad (3.8)$$

We note that $\rho_{A_1 \cup A_2}^\pm$ is unitary equivalent to $\tilde{\rho}_{A_1 \cup A_2}$, indeed $a_{A_2}^\dagger \rho_{A_1 \cup A_2}^\pm = \tilde{\rho}_{A_1 \cup A_2} a_{A_2}^\dagger$. And they have the same spectrum as $\rho_{A_1 \cup A_2}$. Eq. (3.8) can be written in compact form in terms of the reduced density matrix in the fermionic representation (cf. Eq. (2.102)), namely

$$\rho_{A_1 \cup A_2}^{fr} = \sum \langle O_1 O_2 \rangle O_1^\dagger O_2^\dagger, \quad (3.9)$$

and introducing the fake density matrix

$$\rho_{A_1 \cup A_2}^{(B_1)} = \frac{\text{Tr}_{B_1 \cup B_2}[\langle \Psi_0 | a_{B_1}^\dagger \rangle]}{\langle a_{B_1}^\dagger \rangle} \quad \text{Tr} \rho_{A_1 \cup A_2}^{(B_1)} = 1, \quad (3.10)$$

where the trace is over the fermionic degrees of freedom $B_1 \cup B_2$ outside of the subsystem and $|\Psi_0\rangle$ is the ground state. This last operator is not a genuine density matrix because, in general, it is not positive semidefinite, as one can argue by substituting, for example, the projector on the ground state $|\Psi_0\rangle \langle \Psi_0|$ with the density matrix

$$|\Psi_0\rangle \langle \Psi_0| - \left( \frac{2}{3} \langle \lambda_A \rangle \langle \lambda_A | \otimes \frac{1}{\sqrt{2}} \rho_A \otimes \frac{1}{\sqrt{2}} \rho_A \right), \quad (3.11)$$

where $|\lambda_A\rangle$ is eigenvector of $\rho_A$ with eigenvalue $\lambda_A < 1$. Indeed this leads to the fake density matrix $2|\lambda_A\rangle \langle \lambda_A| - \rho_A$.

Because the string $a_{A_2}^\dagger$ commutes with the operators consisting of an even number of Majorana fermions in the block $A_2$, anticommuting, instead, when the number is odd, Eq. (3.8) can be written as follows:

$$\rho_{A_1 \cup A_2}^{fr} = \frac{\rho_{A_1 \cup A_2}^{fr} + a_{A_2}^\dagger \rho_{A_1 \cup A_2}^{fr} a_{A_2}^\dagger}{2} \pm \langle a_{B_1}^\dagger \rangle \frac{\rho_{A_1 \cup A_2}^{fr} - a_{A_2}^\dagger \rho_{A_1 \cup A_2}^{fr} a_{A_2}^\dagger}{2}. \quad (3.12)$$

Observe also that the equations above, in particular Eq. (3.7) and Eq. (3.12), are completely general, that is to say they hold for any spin-$\frac{1}{2}$ chain. They are, however, particularly useful when the system has a free-fermion representation. We have already seen that, in this case, the fermionic RDM is Gaussian (cf. Eq. (2.103)). Actually, all terms of the sum in Eq. (3.12) are indeed Gaussian. This is a consequence of the fact that the algebra of the exponentials of a quadratic form is closed, as we are seeing in the next section.

Here some remarks about the interpretation of (3.12). The operators $\rho_{A_1 \cup A_2}^\pm$ are the RDMs in the fermionic representation of the states

$$|\Psi_{\pm}\rangle = \left( \frac{1}{2} a_{B_1}^\dagger \pm \frac{1}{2} a_{B_1}^\dagger a_{A_2}^\dagger \right) |\Psi_0\rangle. \quad (3.13)$$

These are the ground states of the Hamiltonians

$$H_{\pm} = \left( \frac{1}{2} a_{B_1}^\dagger \pm \frac{1}{2} a_{B_1}^\dagger a_{A_2}^\dagger \right) \hat{H} \left( \frac{1}{2} a_{B_1}^\dagger + \frac{1}{2} a_{B_1}^\dagger a_{A_2}^\dagger \right). \quad (3.14)$$
The unitary transformation above is nontrivial only for operators on the contact surface between the blocks and the remaining chain. Summarizing, we can write a fermionic RDM equivalent to the spin RDM at the price of adding a finite number of non local terms to the Hamiltonian $H$.

Eq. (3.12) is the main result of this section: the representation of the spin RDM as a linear combination of four fermionic RDMs, which are exponentials of a quadratic form (as in Eq. (2.103)) wherever the model can be mapped into free fermions. These four matrices do not commute and so they can not be diagonalized simultaneously to find all eigenvalues of the spin RDM. However, if we are interested in R\'enyi entropies with integer $\alpha$, we can handle this problem in a constructive way: we determine the product rules between RDMs and then we construct recursively any finite order R\'enyi entropy.

### 3.1.1 Product rule

In this subsection we show that, if the system is in the ground state of a “non-interacting” model like the XY model, Eq. (3.12) is sum of 4 Gaussians. Three are the fundamental observations:

- the trace of a fermionic Gaussian operator over some fermionic degrees of freedom is still Gaussian;
- the non-local part of the JW transformation, i.e. the string of $\sigma_z$, and in particular $a_{B_1}^z$, is Gaussian;
- the algebra of fermionic Gaussian operators is closed.

The first observation is consequence of the Wick theorem, being equivalent to the fact that if the correlation functions factorize in two-point fermionic correlations for the total system, then this happens in particular when a restricted number of fermions is considered. The second observation can be easily verified; indeed we find

$$\sigma_i^z = -ia_i^z a_i^\dagger = i e^{\frac{\pi}{2} a_i^x a_i^y},$$

so that any string of $\sigma_z$ is the exponential of a quadratic form. Notice, however, it is not Hermitian. To understand the third observation, we analyze the algebra of RDMs generated by a quadratic form, i.e.

$$\rho_W = \frac{1}{Z(W)} \exp\left(\sum_{l,n} a_l W_{ln} a_n / 4\right),$$

where we do not assume $W$ to be hermitian (to include the non-hermitian contribution of the string). Anti-commutation relations of Majorana operators make always $W$ a complex skew-symmetric matrix, i.e. $W^T = -W$. The constant

$$Z(W) = \text{Tr} \exp\left(\sum_{l,n} a_l W_{ln} a_n / 4\right),$$

53
ensures the normalization $\text{Tr}\rho_W = 1$. In Ref. [9] it is shown that this normalization for complex diagonalizable skew-symmetric matrices is

$$Z(W) = \prod_{\{w\}/\pm} 2 \cosh \left( \frac{w}{2} \right), \quad (3.18)$$

where $\{w\}/\pm$ is the set of eigenvalues of $W$ with halved degeneration ($W$ is a skew-symmetric matrix so any even function of $W$ has eigenvalues with even degeneracy). Here we are assuming $Z(W) \neq 0$.

The product of fermionic RDMs of the form (3.16) is

$$\rho_W \rho_{W'} = \frac{Z(\log(\exp(W) \exp(W')))}{Z(W)Z(W')} \rho_{\log(\exp(W) \exp(W'))}. \quad (3.19)$$

Indeed the commutator of operators in the exponent of (3.16)

$$\sum_{l,n,j,k} W_{ln} W'_{jk} \frac{1}{16} \left[ a_l a_n, a_j a_k \right] = \frac{\vec{a}^T [W, W'] \vec{a}}{4}. \quad (3.20)$$

is the essential ingredient in the Baker-Campbell-Hausdorff formula for the product of exponential of operators. And because any commutator can be moved from the Majorana operators to the matrices $W$ (Eq. (3.20)), we get (3.19).

Fermionic RDMs are specified by the correlation matrices

$$\Gamma_{ij} = \text{Tr}[a_i \rho_W a_j] - \delta_{ij}, \quad (3.21)$$

which can be written as (see, for example, the Appendix of Ref. [9] for a proof valid also when $W$ is not Hermitian)

$$\Gamma = \tanh \left( \frac{W}{2} \right) \quad \Rightarrow \quad e^W = \frac{1 + \Gamma}{1 - \Gamma}. \quad (3.22)$$

Clearly the second equation is true only when $1 - \Gamma$ is an invertible matrix. At this point, let us briefly summarize the logic of the following derivation. We can easily calculate/manipulate the correlation matrix $\Gamma$ that via Eq. (3.22) gives the exponential factor $W$ that defines the quadratic density matrix in Eq. (3.16). We need to find what are the consequences of the product rule of RDMs for the correlation matrices, i.e. we need to find what is the correlation matrix corresponding to the product of two RDMs. While, through the chains of equations above, any $W$ defines a single $\rho_A$, the opposite is not true and there are several possible $W$’s for each $\rho_A$. Nevertheless, we can give a unique recipe for the composition of correlation matrices.

We indicate this matrix operation with $\Gamma \times \Gamma'$ (notice it is not the product of the matrices) and it is formally defined by Eq. (3.19) as

$$\rho[\Gamma] \rho[\Gamma'] = \text{Tr} [\rho[\Gamma] \rho[\Gamma']] \rho[\Gamma \times \Gamma']. \quad (3.23)$$

To specify this operation we still need two ingredients:
3.1 RDM of disjoint blocks in XY chains

1. an usable expression for the correlation matrix

\[(\Gamma \times \Gamma')_{ij} = \frac{Z(W)Z(W')}{Z(\log(\exp(W)\exp(W')))} \text{Tr}_{ia} \rho_W \rho_{W'} a_i - \delta_{ij}, \tag{3.24}\]

associated to the product \(\rho_W \rho_{W'} \equiv \rho[\Gamma] \rho[\Gamma'];\)

2. an expression for the trace of two fermionic RDMs

\[\{\Gamma, \Gamma'\} \equiv \text{Tr}_\rho[\Gamma] \rho[\Gamma'] = \frac{Z(W)Z(W')}{Z(\log(\exp(W)\exp(W')))}, \tag{3.25}\]

in terms of the correlation matrices \(\Gamma\) and \(\Gamma'.\)

The first requirement is easily obtained if we assume \(1 - \Gamma\) and \(1 - \Gamma'\) invertible. Indeed, if we make explicit the exponential products

\[
\frac{1 + \Gamma \times \Gamma'}{1 - \Gamma \times \Gamma'} = \frac{1 + \Gamma 1 + \Gamma'}{1 - \Gamma 1 - \Gamma'}, \tag{3.26}
\]

after simple algebra we obtain

\[
\Gamma \times \Gamma' = 1 - (1 - \Gamma) \frac{1}{1 + \Gamma} (1 - \Gamma'). \tag{3.27}
\]

\(\Gamma \times \Gamma'\) is a skew-symmetric matrix, even if it is not obvious from the formula above. We checked that this relation remains true also if \(1 - \Gamma\) is not invertible (at least for the kind of matrices we are interested in).

The second request is less trivial because the correlation matrix \(\Gamma\) does not determine univocally the matrix \(W\), and the sign of \(Z(W)\) remains ambiguous. However, \(\{\Gamma, \Gamma'\}\) is a functional of \(\Gamma\) and \(\Gamma'\), i.e. it is the product of the eigenvalues of \((1 + \Gamma \Gamma')^{-1}\) with halved degeneration (the spectrum of \(\Gamma \Gamma'\) is double degenerate \([68]\))

\[
\{\Gamma, \Gamma'\} = \prod_{\mu \in \text{Spectrum}[\Gamma \Gamma']/2} \frac{1 + \mu}{2} = \pm \sqrt{\det \frac{1 + \Gamma \Gamma'}{2}}, \tag{3.28}
\]

The unspecified \(\pm\) sign in front is the ambiguity that can be solved by rewriting the composition rule as \([9]\)

\[
\{\Gamma, \Gamma'\} = \exp \left( \frac{1}{2} \int_{\gamma[0 \rightarrow 1]} \frac{d\lambda}{1 + \lambda} \text{Tr} \left( \frac{\Gamma \Gamma' - 1}{\lambda \Gamma \Gamma' + 1} \right) \right), \tag{3.29}
\]

which does not depend on the curve \(\gamma\). In fact, for numerical computations, the first equality in Eq. \((3.28)\) is all we need.

It is evident that the operation \(\times\) is associative and so we are in position to make any product of fermionic RDMs:

\[
\prod_{i=1}^{n} \rho[\Gamma_i] = \{\Gamma_1, \cdots, \Gamma_n\} \rho[\Gamma_1 \times \cdots \times \Gamma_n], \tag{3.30}
\]
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where

\[ \{\Gamma_1, \Gamma_2, \Gamma_3, \ldots, \Gamma_n\} \equiv \text{Tr}[\rho[\Gamma_1]\rho[\Gamma_2] \cdots] = \{\Gamma_1, \Gamma_2\} \{\Gamma_1 \times \Gamma_2, \Gamma_3 \ldots, \Gamma_n\}. \] (3.31)

If, for some \(i\) and \(j\), the matrix \((1 + \Gamma_i \Gamma_j)/2\) is not invertible, Eq. (3.30) cannot be applied, and some ad hoc procedures must be used, as discussed, in part, in the next section.

Summarizing, the trace of the products of fermionic Gaussian operators is given by Eq. (3.31), which is a recursive equation that can be solved easily, as long as the number of factors is not too large. This observation, together with the fact that the RDM is sum of a fixed number (namely 4) of Gaussians, opens the door to the computation of the Rényi entropies with integral index \(\alpha\). Indeed \(\alpha\) will determine the number of RDMs that must be multiplied.

3.1.2 Rényi entropies

From equations (3.7), (3.12) and (3.30), the Rényi entropies for integer \(\alpha\) can be written as follows

\[ S_\alpha = \log \frac{\text{Tr}\rho^\alpha}{1 - \alpha} = \frac{1}{1 - \alpha} \log \left[ \frac{1}{2^\alpha} \sum_{\zeta_1, \ldots, \zeta_\alpha} \prod_{i=1}^\alpha c[\zeta_i] \{\Gamma_{\zeta_1}, \ldots, \Gamma_{\zeta_\alpha}\} \right], \] (3.32)

where we defined the variables \(\zeta_i = 1, 2, 3, 4\) (that label which of the terms in Eq. (3.32) is taken in the particular product) and we defined the shorts for the 2-point correlation matrices (in the following all density matrices refer to the subsystem \(A_1 \cup A_2\))

\[ \Gamma_1 = \Gamma_{\rho^{fer}}, \quad \Gamma_2 = \Gamma_{a_A^{z_B} \rho^{az_A} a_A^{z_B}}, \quad \Gamma_3 = \Gamma_{\rho^{(B_1)}}, \quad \Gamma_4 = \Gamma_{a_A^{z_B} \rho^{(B_1)} a_A^{z_B}}, \] (3.33)

and

\[ c[\zeta] = \begin{cases} 1 & \zeta \in \{1, 2\} \\ \langle a_B^{\zeta} \rangle & \zeta = 3 \\ -(a_B^{\zeta}) & \zeta = 4. \end{cases} \] (3.34)

In the case of \(\alpha = 2\) the above expression can be rewritten as

\[ S_2 = -\log \frac{1}{4} \sum_{\zeta_1, \zeta_2} c[\zeta_1] c[\zeta_2] (\pm) \sqrt{\det \left| \frac{1 - \Gamma_{\zeta_1}}{2} \frac{1 - \Gamma_{\zeta_2}}{2} + \frac{1 + \Gamma_{\zeta_1}}{2} \frac{1 + \Gamma_{\zeta_2}}{2} \right|}, \] (3.35)

where here and in the following equation we leave the sign ambiguity unspecified. Taking into account the trace’s invariance under cyclic permutations, \(S_2\) becomes the logarithm of a sum of 10 terms

\[ \text{Tr}\rho^2 = \frac{1}{4} \sum_{\zeta} c[\zeta]^2 \sqrt{\det \left| \frac{1 + \Gamma_{\zeta}^2}{2} \right|} + \frac{1}{2} \sum_{\zeta_1 > \zeta_2} c[\zeta_1] c[\zeta_2] (\pm) \sqrt{\det \left| \frac{1 - \Gamma_{\zeta_1}}{2} \frac{1 - \Gamma_{\zeta_2}}{2} + \frac{1 + \Gamma_{\zeta_1}}{2} \frac{1 + \Gamma_{\zeta_2}}{2} \right|}. \] (3.36)

These formulae are already usable for a direct computation of Rényi entropies. There are however some simplifications that occur by using the property of the correlation matrices \(\Gamma\)’s.
The first matrix $\Gamma_1$ is the standard fermionic correlation matrix (i.e. the one corresponding to free fermions in the absence of the Jordan-Wigner string, already considered in Ref. [69]). $\Gamma_2$ can be obtained from $\Gamma_1$ as $\Gamma_2 = (P_2 \otimes I_2)\Gamma_1(P_2 \otimes I_2)$, with $P_2$ the Hermitian unitary matrix

$$P_2 \equiv \begin{pmatrix} I_{A_1} & 0 \\ 0 & -I_{A_2} \end{pmatrix},$$  \hspace{1cm} (3.37)$$

and $I_2$ the $2 \times 2$ identity matrix representing the space of the two Majorana fermions defined in each site. The same relation occurs between the third and the forth matrix $\Gamma_4 = (P_2 \otimes I_2)\Gamma_3(P_2 \otimes I_2)$. Instead $\Gamma_3$ is not trivially related to $\Gamma_1$. In Ref. [9] we have proved the following identity

$$\Gamma_3 = \Gamma_1 - \Gamma_{AB} \Gamma_{B_1 B_2} \Gamma_{B_2 B_1},$$  \hspace{1cm} (3.38)$$

where the double subscripts take into account restrictions to rectangular correlation matrices, i.e. the first (second) subscript identifies the region where the row (column) index runs. In Sec. 3.6 we show that similar properties are valid also for an arbitrary number of intervals.

Using these relations after some algebraic manipulations one can write down the full sums for the R"enyi entropies. It is important to notice that $\langle a \bar{b}_1 \rangle = \sqrt{n} \text{Pf}(\Gamma_{B_1})$ and so $\langle a \bar{b}_1 \rangle^2 = (-1)^n \det(\Gamma_{B_1}) = | \det \Gamma_{B_1} |$. Furthermore to short the notations we write sequences of identical correlation matrices in the compact form:

$$\{ \cdots, \Gamma_i^n, \cdots \} = \{ \cdots, \underbrace{\Gamma_i \cdots \Gamma_i}_n \cdots \}.$$  \hspace{1cm} (3.39)$$

Finally $S_2$ can be written in a rather simple way

$$S_2 = -\frac{1}{2} \log \left[ \frac{\{\Gamma_1^2\} + 3\{\Gamma_1, \Gamma_2\}}{2} + | \det \Gamma_{B_1} | \frac{\{\Gamma_3, \Gamma_4\} - \{\Gamma_3, \Gamma_4\}}{2} \right].$$  \hspace{1cm} (3.40)$$

But, increasing the order $\alpha$, the explicit expressions become soon long. For example, here are the (simplified) formulae for $S_3$

$$S_3 = -\frac{1}{2} \log \left[ \frac{\{\Gamma_1^4\} + 3\{\Gamma_1^2, \Gamma_2\} + 3| \det \Gamma_{B_1} | \{\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4\}}{4} \right],$$  \hspace{1cm} (3.41)$$

and $S_4$

$$S_4 = -\frac{1}{3} \log \left[ \frac{\{\Gamma_1^4\} + 4\{\Gamma_1^3, \Gamma_2\} + 2\{\Gamma_1^2, \Gamma_3, \Gamma_4\} + \{\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4\}}{8} \right] + | \det \Gamma_{B_1} | \left( \frac{\{\Gamma_1, \Gamma_3, \Gamma_4\} + \{\Gamma_1, \Gamma_4, \Gamma_3, \Gamma_4\}}{4} + \frac{\{\Gamma_1, \Gamma_3, \Gamma_4\} + \{\Gamma_1, \Gamma_4, \Gamma_3, \Gamma_4\}}{2} \right) + \frac{\{\Gamma_1, \Gamma_3, \Gamma_2, \Gamma_4\}}{2} - \frac{\{\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4\}}{2} + \frac{\{\Gamma_1, \Gamma_2, \Gamma_4, \Gamma_3\}}{2} - \frac{\{\Gamma_3, \Gamma_4, \Gamma_2, \Gamma_1\}}{2} + \frac{\{\Gamma_3, \Gamma_4, \Gamma_3, \Gamma_4\}}{2} + \frac{\{\Gamma_3, \Gamma_4, \Gamma_3, \Gamma_4\}}{2} + \frac{\{\Gamma_3, \Gamma_4, \Gamma_3, \Gamma_4\}}{2} + \frac{\{\Gamma_3, \Gamma_4, \Gamma_3, \Gamma_4\}}{8}. $$
We stress that if \( \det \Gamma_{B_1} = 0 \), i.e. \( \langle a^2_{B_1} \rangle = 0 \), we can not simplify the terms multiplied by \( \det \Gamma_{B_1} \). This is because they are divergent, and the expressions are indeterminate. Actually, these indeterminateness can be easily cured. In fact, in the recursive expansion (3.31) one could isolate the problematic terms

\[
Pf(\Gamma_{B_1}) \{ \Gamma_3, \Gamma' \} = Pf \left( \Gamma_{B_1} - \Gamma_{B_1} A \frac{1}{1 + \Gamma_{1}} \Gamma_{AB_1} \right) \]

where the equalities above follow from the chain of identities

\[
\det D \det(A - BD^{-1}C) = \det A \det(D - CA^{-1}B) = \det \begin{pmatrix} A & B \\ C & D \end{pmatrix},
\]

The right hand sides of Eqs. (3.43) have no apparent divergences due to the inversion of \( \Gamma_{B_1} \). For the sake of simplicity we assume \( \{ \Gamma_1, \Gamma' \} \neq 0 \) (this is indeed the case for the configurations considered here), otherwise also other terms involving only \( \Gamma_1 \) and \( \Gamma_2 \) would be problematic. However, such problems can be always overcome by increasing the size of the matrices. For example, if \( \{ \Gamma, \Gamma' \} = 0 \), the expression

\[
\{ \Gamma, \Gamma', \Gamma'' \} = \{ \Gamma, \Gamma' \} \{ \Gamma \times \Gamma', \Gamma'' \}
\]

is not well-defined (\( \Gamma \times \Gamma' \) involves the inverse of a non-invertible matrix). However, from the last identity of Eq. (3.44) we see that the l.h.s. of Eq. (3.45) can be rewritten as

\[
\{ \Gamma, \Gamma', \Gamma'' \} = \pm \sqrt{\det \left| \frac{1}{2} I + \left( I - \Gamma \frac{1}{2} \right) \left( \frac{1}{2} \Gamma' 0 \\ 0 1 \right) \right|},
\]

which instead has no divergences. Notice that if \( \langle a^2_{B_1} \rangle \) vanishes, the matrix \( \Gamma_3 \) in Eq. (3.38) is not well-defined, however the following equivalent definition can be employed:

\[
\Gamma_3 = (\Gamma_1 + iI_A) \Gamma_1 + iI_A + \Gamma_{AB_1} (\Gamma_{B_1}, B_1 - \Gamma_{B_1} A (\Gamma_1 + iI_A)^{-1})^{-1} \Gamma_{B_1} A (\Gamma_1 + iI_A) - iI_A
\]

The general method to tackle indeterminateness is by using Eq. (3.44) and the Woodbury identity

\[
\frac{1}{A^{-1} + UC^{-1}V} = A - AU \frac{1}{C + VAU} V A,
\]

in order to deal with well-defined objects.

In the paragraph below we analyze the simplifications that occur considering the XX model. Incidentally, we run up against the troubles discussed above, indeed \( \det \Gamma_{B_1} = 0 \) when the magnetic field \( h = 0 \).
3.1 RDM of disjoint blocks in XY chains

**XX model.** The isotropic XY model is the prototype of systems that conserve the number of JW fermions. The correlation matrix $\Gamma$ between Majorana fermions is factorized (cf. Eq. (2.44))

$$\Gamma_1 \sim (1 - 2C_1) \oplus (2C_1^T - 1),$$

where $C_{ln} = \langle c_l^\dagger c_n \rangle$ is an $\ell_A \times \ell_A$ Hermitian matrix. In addition we find that the correlation matrix of the fake reduced density matrix $\rho(B_1)$ is given by

$$\Gamma_3 \sim (1 - 2C_3) \oplus (2C_3^T - 1) \quad \text{with} \quad C_3 = C_1 - C_{AB_1}(C_{B_1B_1} - \frac{1}{2}I_{B_1})^{-1}C_{B_1A}.$$

The definitions of $C_2$ and $C_4$ follow immediately: $C_2 = P_2C_1P_2$, $C_4 = P_2C_3P_2$. The $\times$-product reads as

$$\Gamma \times \Gamma' = (1 - 2C \times C') \oplus (2(C \times C')^T - 1),$$

where the $\times$-product for the correlation matrices $C$ is defined as follows:

$$C \times C' = C'(1 - C - C' + 2CC')^{-1}C.$$

The factorization still remains when the correlation matrices are multiplied among themselves, and hence

$$\{\Gamma_1, \Gamma_2, \Gamma_3, \ldots, \Gamma_n\} \equiv \{C_1, C_2, C_3, \ldots, C_n\} = \{C_1, C_2\}\{C_1 \times C_2, C_3, \ldots, C_n\},$$

with

$$\{C_1, C_2\} = \det|1 - C_1 - C_2 + 2C_1C_2|.$$

The configurations in which $\langle a^\dagger_{B_1} a_{B_1} \rangle = 0$, e.g. in the absence of magnetic field, can be taken into account by using Eqs. (3.43) in which $\Gamma \rightarrow 1 - 2C$, pfaffians become determinants, and determinants are squared.

In conclusion, we have developed a formalism for calculating the first integer Rényi entropies in models with a free-fermion representation. Unfortunately, we didn’t find the Rényi entropies in closed form, and our method is unsuitable for calculating the entropies for large values of $\alpha$. Furthermore, we don’t know how to perform the analytic continuation as $\alpha$ approaches 1, in order to get the entanglement entropy. In fact these problems are also found in the CFT calculations so that, up to now, nor analytic expressions, neither exact numerical calculations exist for the von Neumann entropy in a large system.

The remainder of the chapter is devoted to review, and checked against numerics, the CFT predictions for the universal functions $F_\alpha(x)$ (see Eq. (3.2)) in the critical XX and Ising models. We also provide semi-analytic results for the Rényi entropies in non-critical systems. Finally, we come back to the von Neumann entropy, exploiting the inequalities (1.24) to get bounds for the universal function $F_{\nu,N}(x) \equiv \lim_{\alpha \rightarrow 1^+} F_\alpha^*(x)$. At the end of the chapter the generalization to many disjoint blocks will be investigated.
3.2 Critical models

In the thermodynamic limit, the Rényi entropies of two disjoint blocks of lengths \(\ell_1\) and \(\ell_2\) at the distance \(r\) in a CFT are given by (cf. Eq. (3.2))

\[
S_\alpha = \frac{1 + \alpha c}{\alpha 6} \log \left( \frac{\ell_1 \ell_2(r + \ell_1 + \ell_2)}{(\ell_1 + r)(r + \ell_2)} \right) + \frac{\log F_\alpha(x)}{1 - \alpha} + \frac{\log c_1^2}{1 - \alpha} \quad x = \frac{\ell_1 \ell_2}{(\ell_1 + r)(r + \ell_2)}. \tag{3.55}
\]

As it happens for a single interval, the divergent part of the Rényi entropies in the limit of infinite lengths depends only on the central charge of the theory. However, the additive factor has a universal part characterized by the function \(F_\alpha(x)\). For the sake of simplicity we assume \(\ell_1 = \ell_2 = \ell\). In considering spin chains, whose continuum limit is conformal, one has to deal with finite blocks’ lengths: corrections to the scaling have to be considered. This means that \(F_\alpha(x)\) in Eqs. (3.2) and (3.55) must be substituted with \(F_\alpha(x,\ell)\), which takes into account the corrections to the scaling

\[
F_\alpha(x,\ell) = F_\alpha(x) + \ell^{-\delta_\alpha} f_\alpha(x) + \ldots. \tag{3.56}
\]

The exponent \(\delta_\alpha\) governs the leading correction. It has been shown with CFT in Ref. [70] that this exponent is equal to \(\frac{2y}{\alpha}\) independently of the number of intervals, and \(y\) is the scaling dimension of an operator that can be relevant, i.e. \(y < 2\). In Chapter 4 we will analyze the corrections to the scaling in the XX model. In the following we survey and check the CFT results for \(F_\alpha(x)\) and \(\delta_\alpha\) in the critical XX and Ising models. In particular we show that the non-triviality of \(F_\alpha(x)\) is deeply related to the structure of Eq. (3.12).

3.2.1 Critical XX model

In this subsection we report the explicit results for the XX chain in zero magnetic field (i.e. Eq. (2.15) with \(h = 0\)). The critical XX model is described by the CFT of a free boson compactified on a circle. The functions \(F_\alpha(x)\) can be written in terms of a universal critical exponent \(\eta\) (defined, e.g., in Ref. [28]) which is proportional to the square of the compactification radius. In particular, in this model it is equal to \(\frac{1}{2}\), and \(F_\alpha(x)\) is given by [14]

\[
F_\alpha(x) = \frac{\Theta(0|\Gamma/2)\Theta(0|2\Gamma)}{[\Theta(0|\Gamma)]^2} \tag{3.57}
\]

where \(\Gamma\) is an \((\alpha - 1) \times (\alpha - 1)\) matrix with elements

\[
\Gamma_{rs} = \frac{2i}{\alpha} \sum_{k=0}^{\alpha-1} \sin \left( \frac{k}{\alpha} \right) \beta_{k/s} \cos \left[ 2\pi \frac{k}{\alpha} (r - s) \right], \tag{3.58}
\]

where

\[
\beta_y = \frac{F_y(1 - x)}{F_y(x)}, \quad F_y(x) = \text{$_2F_1(y, 1 - y, 1, x)$} \tag{3.59}
\]
and $\Theta$ is the Riemann-Siegel theta function

$$\Theta(z|\Gamma) = \sum_{m \in \mathbb{Z}} \exp\left[i\pi m^t \cdot \Gamma \cdot m + 2\pi im^t \cdot z\right],$$  \hspace{1cm} (3.60)

with $z$ a generic complex vector of $\alpha - 1$ components. The expression (3.57) can be written in terms of elementary functions for specific values of $\alpha$: e.g. for $\alpha = 2$ we get

$$F_2(x) = \sqrt{(1 + \sqrt{1 - x})(1 + \sqrt{x})}.$$ \hspace{1cm} (3.61)

XX chains have been previously analyzed by Furukawa et al in Ref. [28] by means of exact diagonalization techniques. The asymptotic results from CFT (cf. Eq. (3.61)) were obscured in this previous analysis by large oscillating corrections to the scaling, being the system sizes too small in order to isolate the universal function $F_\alpha(x)$ from $F_\alpha(x,\ell)$ (see Eq. (3.56)). The smallness of the systems and the lack of a precise knowledge of the form of the correction to the scaling made impossible any finite-size scaling analysis to check the CFT predictions (3.61). A precise theory about the origin and the exact form of these oscillations is only recently available [70,71].

By exploiting the exact solution, in Ref. [9] we were able to avoid these problems and explore large enough values of $\ell$ allowing a finite-\ell scaling analysis similar to the one for a single block [71]. We start from the infinite volume limit. For a single interval we will see in Chapter 4 that the exponent $\delta_\alpha$ of the corrections to the scaling (Eq. (3.56)) is equal to $2/\alpha$ [71], manifesting the presence of a relevant operator with scaling dimension $x = 1$, which has been justified in Ref. [70]. The existence of such an operator influences the corrections to the scaling of the entanglement entropies for any number of intervals and hence we expect the same exponent for the double interval case.

We report in Fig. 3.2 results for the function $F_{2,3,4}^{\text{lat}}(x,\ell)$ for various $\ell$ and $x$. It is evident that irrespective of the value of $x$, with increasing $\ell$ the results approach the CFT prediction. For odd $\ell$ the asymptotic result is approached from below, while for even ones it is approached from above. These are the already mentioned oscillations that made difficult the analysis based on small chains. These plots confirm the correctness of Eq. (3.57): the figures do not leave doubts about the correctness of the CFT results of Ref. [14]. It is worth to mention that the finite $\ell$ curves do not have the symmetry $x \rightarrow 1 - x$ that is restored only in the $\ell \rightarrow \infty$ limit Eq. (3.57). This is partially due to the definition (3.55), which is not manifestly invariant under interchanging subsystem with the rest (the formula holds only if all lengths are much less than the chain’s length). A little improvement in this direction could be done by rewriting the first piece of Eq. (3.57) in terms of the Renyi entropies of the blocks

$$S_\alpha^{[A_1 \cup A_2]} = S_\alpha^{[A_1]} + S_\alpha^{[A_2]} + S_\alpha^{[B_1]} + S_\alpha^{[A_1 \cup B_1 \cup A_2]} - S_\alpha^{[A_1 \cup B_1]} - S_\alpha^{[B_1 \cup A_2]} + \frac{\log F_\alpha}{1 - \alpha},$$ \hspace{1cm} (3.62)

however $\ell_{1(2)}$ is not invariant under the transformation so that the curves, at $\ell$ fixed, remain asymmetric. We analyze in more details the issue of recovering such symmetry in Sec. 3.5.
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Figure 3.2: $F_\alpha$ in the critical XX model - Scaling function $F^{\text{lat}}_\alpha(x)$ for $\alpha = 2, 3, 4$ (from top to bottom) for the XX model in the thermodynamic limit and for various $\ell = \ell_1 = \ell_2$ and $r$. Corrections to the scaling show even-odd oscillations with $\ell$ as in the single interval case. The results converge quickly to the universal CFT prediction $F_\alpha(x)$. 
Here, we continue to work with the definition (3.55) to be consistent with the previous works. Having established the correctness of the asymptotic form, we can now move to the finite \( \ell \)
corrections and check whether the prediction \( \delta_\alpha = 2/\alpha \) is correct. Having precise control of the corrections to the scaling is not an academic task: their analysis is fundamental to provide accurate results when such large system sizes are not available and in cases when the asymptotic form is not known. In Fig. 3.3, we report the function \( |F_\alpha(x) - F_{\text{flat}}(x)| \) for fixed \( x = 1/9 \) and \( \alpha = 2, 3, 4 \). We both report results for the spin R\'enyi entropies and for the fermionic ones (i.e. those corresponding to the RDM in the fermionic representation \( \rho_{A_1 \cup A_2}^{\text{fer}} \), without considering the string contribution).

We recall that for free fermions we have \( F_\alpha(x) = 1 \) identically [72]. The results show a power law behavior for large enough \( \ell \) with the predicted exponent \( 2/\alpha \) as for the single interval. Notice that, by increasing \( \alpha \), the values \( \ell \) where the leading asymptotic correction can be identified become larger and larger, in analogy with the single block case (as obvious because
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of the smallness of the exponent $\delta_\alpha$). For the fermionic variables the asymptotic behavior is reached before than for spin degrees of freedom: the string $a^2_{\beta_1}$ introduces further corrections to the scaling that in the present model are subleading. To show the $x$ independence of this exponent in the last panel of Fig. 3.3, we report the same kind of plots for different values of $x$, showing that, at fixed $\alpha$, the corrections lie on parallel lines.

To conclude this subsection we present some results for finite systems. In fact the prescription to replace the distances by the chord lengths as in the single interval case \((1.58)\) still hold for disjoint blocks. Thus, the leading order in finite systems can be described by replacing any distance $u_{ij}$ by the chord length $u_{ij} \to \frac{L}{\pi} \sin \frac{\pi u_{ij}}{L}$ in all the formulae above (including in the expression of the four-point ratio $x$ Eq. \((3.55)\)). We only show the results for a rather small system of length $L = 39$ (that nevertheless is above anything obtainable by exact diagonalization). In Fig 3.4 we report the resulting $F^2_{\text{lat}}$ for all the possible divisions in four parts of this chain of length $L = 39$. For such small chain, the results are obviously very unclear since the corrections to the scaling are obscuring the CFT scaling represented by a continuous line that is surrounded by the points, signaling the oscillatory nature of the corrections (for clarity, compare with the analogous plot for the Ising model in next section).

![Figure 3.4: General picture of $F^2_{\text{lat}}(x)$ in the critical XX model - The function $F^2_{\text{lat}}(x)$ for a small chain with $L = 39$ spins. Oscillating corrections to the scaling prevent to see the universal CFT prediction shown as a continuous curve.](image-url)
3.2 Critical models

Figure 3.5: $F_\alpha$ in the critical Ising model - Scaling function $F^{\text{lat}}_\alpha(x)$ for $\alpha = 2, 3, 4$ (from top to bottom) for the Ising model in the thermodynamic limit and for various $\ell$. Corrections to the scaling are monotonous. The top curve in each plot is the extrapolation to $\ell \to \infty$. The convergence to the universal CFT prediction $F_\alpha(x)$ is slower than in the XX case, because the leading exponent of corrections to the scaling is $1/\alpha$. 
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3.2.2 Critical Ising universality class

The Ising model is given by the Hamiltonian (2.12) and it is critical for $h = 1$. The universal functions $F_{\alpha}(x)$ in the Ising universality class are given by [27]

$$F_{\alpha}(x) = \frac{1}{2^{\alpha-1} \Theta(0, \Gamma)} \sum_{\epsilon, \delta} \left| \Theta^{[\epsilon]}_{[\delta]}(0|\Gamma) \right|$$  \(3.63\)

where $\Gamma$ is the same as in (3.58) and $\Theta$ is the Riemann theta function with characteristic defined as

$$\Theta^{[\epsilon]}_{[\delta]}(0|\Gamma) = \sum_{m \in \mathbb{Z}^{\alpha-1}} \exp \left[ i\pi (m + \epsilon)^T \cdot \Gamma \cdot (m + \epsilon) + 2\pi i (m + \epsilon)^T \cdot (z + \delta) \right], \quad \Theta(0, \Gamma)$$  \(3.64\)

with $z$ a generic complex vector of $\alpha - 1$ components. The sum is intended over all $2^{\alpha-1}$ vectors $\epsilon$ and $\delta$ with entries 0 and 1/2. The expression (3.63) can be written in terms of elementary functions for specific values of $\alpha$: e.g. for $\alpha = 2$ we get

$$F_2(x) = \frac{1}{\sqrt{2}} \left( \sqrt{\frac{(1 + \sqrt{1 - x})(1 + \sqrt{x})}{2}} + x^{\frac{1}{4}} + \sqrt{x(1-x)^{\frac{1}{4}} + (1-x)^{\frac{1}{4}}} \right). \quad (3.65)$$

Results for this model have been firstly derived numerically for $\alpha = 2$ in Ref. [67] by using a tree tensor network algorithm and Monte Carlo simulations of the two-dimensional classical problem in the same universality class. These calculations allowed a precise determination of $F_2(x)$, but the system sizes explored were not enough to analyze Rényi entropies with larger values of $\alpha$.

We report the results that we have obtained in the thermodynamic limit for various values of $\ell = \ell_1 = \ell_2$ at different separations $r$ (resulting in the four-point ratio $x$ given in Eq. (3.55)) in Fig. 3.5. Oppositely to the XX chain, in the Ising model we have monotonic finite $\ell$ corrections to the scaling. For finite $\ell$, the results do not show the symmetry $x \to 1 - x$ valid for infinite $\ell$. This is restored only by the extrapolated data at $\ell \to \infty$. To perform this extrapolation in the most accurate way, we have first to determine the exponent of the correction. For a single interval, it is exactly known that the leading corrections are characterized by the exponent $\delta_{\alpha} = 2/\alpha$ as for the XX chain. However for $\alpha = 2$, it has been shown in Ref. [67] that $\delta_2 = 1/2$, different from the single interval one. This result is quite surprising also in view of the CFT analysis [70] predicting the same behavior for any number of intervals. By exploiting our formalism, we can check the exponent of the corrections to the scaling for the Ising model in the absence of the Jordan-Wigner string between the two blocks $\hat{a}_{B_1}^\dagger$ (i.e. we consider only the correlation matrix $\Gamma_1$, as done in Ref. [69]). In this case, the results reported in Fig. 3.6 give a compelling evidence that the leading corrections to the scaling are given by $\delta_{\alpha} = 2/\alpha$ as in the single interval. In fact, the Jordan-Wigner string produces another operator at the conical singularity, that in the Ising model is the leading one. According to Ref. [70] all the corrections to the scaling should be of the form $\delta_{\alpha} = 2y/\alpha$, thus taking the result $\delta_2 = 1/2$ for granted, we conclude that the Jordan-Wigner string $\hat{a}_{B_1}^\dagger$ introduces an operator with scaling
3.2 Critical models

Figure 3.6: Fermionic corrections to the scaling \( F_{2}^{\text{Ferm}}(x) \) for different \( x \) and \( \gamma \). All results present the same leading correction to the scaling exponent \( \delta_2 = 1 \). The extrapolated data at \( \ell \to \infty \) collapse in the single point \( F_2(x) = 1 \).

Dimension \( y = 1/2 \). Such an operator in the continuum limit of the Ising model exists and it is the Majorana fermion, that has exactly the same features of the Jordan-Wigner string (i.e. same symmetry and same non-local character). Such an operator is clearly not present in the single interval case. These considerations allow to conclude that the leading corrections to the scaling for the double interval entanglement in the Ising model are described by the exponent

\[
\delta_\alpha = \frac{1}{\alpha}.
\]

Unfortunately already for \( \alpha = 3 \), the value of \( \delta_3 = 1/3 \) is very low and subleading corrections to the scaling going with exponents \( m\delta_\alpha \) (with \( m \) integer) are expected to influence the results in a considerable manner. For this reason, in order to have an accurate determination of the asymptotic behavior, at fixed \( x \) we consider all corrections to the scaling up to those with exponent 1. The resulting extrapolated data are the top points in Fig. 3.5. For \( \alpha = 2, 3, 4 \) the CFT predictions \( F_{2,3,4}(x) \) (cf. Eq. (3.65) and Eq. (3.63) with \( \alpha = 3, 4 \)) perfectly with the extrapolated data agree, giving strong support both for the procedure to account for the subleading corrections terms and for the asymptotic form.

We now turn to consider the issue of universality. All the critical models \((h = 1)\) for any value of \( \gamma \neq 0 \) are in the Ising universality class. However, the results at finite \( \ell \) show a strong dependency on \( \gamma \) (as obvious from the different correlation matrices). In Fig. 3.7 we report several data for \( F_2^{\text{lat}}(x) \) for different values of \( \gamma \) and \( \ell \) at fixed \( x = 1/4 \) and \( x = 3/4 \) (that for the symmetry \( x \to 1 - x \) have the same asymptotic value). At finite \( \ell \), all results are
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Figure 3.7: Universality with respect to $\gamma$ - We plot $F^\text{lat}_2(x)$ for $x = 1/4$ and $x = 3/4$ for different values of $\gamma$ in the Hamiltonian. All results present the same leading correction to the scaling exponent $\delta_2 = 1/2$. The extrapolated data at $\ell \to \infty$ collapse in a single point equal to $F_2(1/4) = F_2(3/4) = 1.31886\ldots$

evidently different. In the figure we report the extrapolation with two corrections to the scaling (i.e. with $\delta_2 = 1/2$ and $2\delta_2$). For $\ell \to \infty$ all data tend to the same value predicted by CFT $F_2(1/4) = (2 + \sqrt{2}(1 + 3^{1/4}))/4$, confirming in a single plot many results: (i) universality with respect to $\gamma$, (ii) correctness of the correction to the scaling form, (iii) correctness of the CFT prediction Eq. (3.65).

To conclude this section we report the data for a finite chain. As usual, in all the scaling variables we substitute distances with the chord distances. In Fig. 3.8 we report the values of $F^\text{lat}_2(x)$ for all the possible choices of intervals $A_{1,2}$ and $B_{1,2}$ in a chain of $L = 39$ spins. Compared to the analogous plot for the XX chain (Fig. 3.4), the figure is much clearer, due to the fact that corrections to the scaling are monotonous. Notice however that the data points lie much below the asymptotic value because the exponent $\delta_2 = 1/2$ is small (also compared to the XX case with $\delta_2 = 1$) resulting in very large corrections to the scaling.

3.3 Non critical models

The richness of the phase diagram of the XY model allows us also to explore gapped phases that are almost everywhere except on the line $|h| = 1$ and the segment $\gamma = 0$ with $h^2 < 1$. In non-critical systems all the correlations and entanglement between the two blocks fall off exponentially (with a decay rate given by the inverse gap or mass). Thus one would always
3.3 Non critical models

Figure 3.8: General picture of $F^{\text{lat}}_2(x)$ in the critical Ising model - The function $F^{\text{lat}}_2(x)$ for a small chain with $L = 39$ spins. Corrections to the scaling are monotonous and very large compared to the XX case: The data lie much below the asymptotic value predicted by CFT.

expect

$$S_{\alpha}(\ell, r, \ell') = S_{\alpha}(\ell) + S_{\alpha}(\ell') + O(e^{-r/\Delta}).$$

(3.67)

However, this is not so obvious because of the importance of the connected part in the correlations. In Fig. 3.9 (left) we report $S_2$ for the double interval case. While for $h > 1$, the spin entropy is the same as the double of the single interval and the same as the fermionic one, for $h < 1$ there is clearly an offset (that we quantify in $-\log 2$, see below). The best way of detecting these unexpected effects is to consider the mutual entropy

$$\Delta S_{\alpha}(\ell, r, \ell') = S_{\alpha}(\ell) + S_{\alpha}(\ell') - S_{\alpha}(\ell, r, \ell'),$$

(3.68)

that gives automatically zero when factorization occurs.

From numerical data we deduce that, for large blocks, all terms

$$\prod_{i=1}^{\alpha} e^{\zeta_i} \{ \Gamma_{\zeta_1}, \cdots, \Gamma_{\zeta_\alpha} \},$$

(3.69)

in Eq. (3.32) have the same absolute value. However, they can have different signs. Furthermore numerical evidence suggests that terms consisting only of the correlation matrices $\Gamma_1$ and $\Gamma_2$ have always positive sign. If these observations are generally true, we have

$$\Delta S_{\alpha} \sim \frac{1}{\alpha - 1} \log \left[ 1 + \frac{1}{2^\alpha} \sum_{\{\zeta\} \neq \emptyset} (-1)^{# \epsilon(\{\zeta\})} \right],$$

(3.70)
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Figure 3.9: $S_2$ for non-critical models - Left: Comparison of the Rényi entropy $S_2$ for a non-critical Ising model of two disjoint intervals versus the double of the single interval and the fermionic one. While the fermionic entropy is asymptotically always the double of the single interval case, the one in spin variables presents a $-\log 2$ difference due to the string. Right: Mutual entropy $\Delta S_2$ as a function of the magnetic field $h$ for an Ising chain of 129 and 257 spins. The crossing at the phase transition is shown for three configurations. The intercept with $h = 1$ is in good agreement with the CFT prediction. The opaque lines are the corresponding fermionic mutual entropies.

where $\epsilon[\zeta]$ is the sign associated to the element $\{\Gamma_{\zeta_1}, \cdots, \Gamma_{\zeta_\alpha}\}$ and $\#_3(4)$ is the number of correlation matrices $\Gamma_3(4)$. We expect an eventual discontinuity in $\Delta S_\alpha$ when crossing a critical line. Thus we study non-critical chains with magnetic field close to $h = 1$. We found numerically that only terms with odd number of correlation matrices $\Gamma_3(4)$ display sign changes. Thus (see right panel of Fig. 3.9 for the explicit plot) we conclude from the numerical evidence, the behavior

$$\Delta S_\alpha = \begin{cases} \log 2 & h^2 < 1 \\ 0 & \text{otherwise}. \end{cases} \quad (3.71)$$

This result is not completely unexpected: also $S_A$ of the single interval for $|h| = 0$ tends to $\log 2$, independently on $\ell$. Thus in the definition of $\Delta S_\alpha$, since also the double interval $S_\alpha$ tends to the same value, we are left with a single $\log 2$.\footnote{This is a consequence of the double degeneration of the ground state for $|h| < 1$. It is easily understood at $h = 0$, where the ground state is any linear combination of the states all up and all down that we can denote with $|\uparrow\rangle$ and $|\downarrow\rangle$. Since there is no symmetry breaking term in the Hamiltonian, the diagonalization selects a state with zero magnetization, i.e. $(|\uparrow\rangle \pm |\downarrow\rangle)/\sqrt{2}$, in which the entanglement of any subsystem, connected or not, is always $\log 2$ as stated in the main text.}

We stress that at $h = 1$ the various $\Delta_\alpha$ cross in a single point if they are characterized by the same four point ratio $x$ (see right panel of Fig. 3.9) that is the CFT prediction. These kind of plots could be used to detect the phase transition points in systems where it is not exactly known.

The $\alpha$ independence of the previous expression, allows us to analytical continue the result to $\alpha = 1$ and to conjecture the same behavior for the asymptotic von Neumann entanglement...
3.4 $F_{v.N.}(x)$: bounds from strong subadditivity

In this section we consider the universal function $F_{v.N}(x)$ corresponding to the Von Neumann entropy of two disjoint blocks in a conformal system

$$S_{v.N.} = \frac{c}{3} \log \left( \frac{\ell_1 \ell_2 (\ell_1 + r + \ell_2)}{(\ell_1 + r)(r + \ell_2) a^2} \right) - F_{v.N}(x) + 2c_1' \quad x = \frac{\ell_1 \ell_2}{(\ell_1 + r)(r + \ell_2)},$$

(3.73)

where $c_1'$ is the same constant of the single interval (cf. Eq. (1.57)). Observe that $F_{v.N.}(0) = F_{v.N.}(1) = 0$. In fact $F_{v.N.}(x)$ is known for no model. In Ref. [27], however, the small $x$ behavior of $F_{v.N.}$ has been obtained:

$$F_{v.N.}(x) = N \left( \frac{x}{4} \right) \frac{\sqrt{\pi} \Gamma(\alpha + 1)}{4\Gamma(\alpha + \frac{3}{2})} + \ldots \quad x \ll \frac{1}{2},$$

(3.74)

where the integer $N$ counts the number of inequivalent correlation functions giving the same contribution: $N = 2$ for the free boson (XX model) and $N = 1$ for the Ising model. The exponent $\alpha$ is equal to $\min(\eta, 1/\eta)$ for the free boson (in particular $\alpha = \frac{1}{2}$ for the XX model) and to $\frac{1}{2}$ for the Ising model [27]. Essentially, this is all it is known about $F_{v.N.}$, up to now.

We attack the problem from a different point of view: we investigate some of the constraints that strong subadditivity (cf. Eq. (1.24))

$$S(\ell_B + \ell_A; \ell_B' + \ell_C) + S(\ell_B; \ell_A + r; \ell_B') \leq S(\ell_B + \ell_A; r; \ell_B') + S(\ell_B; \ell_A + r; \ell_B' + \ell_C),$$

$$S(\ell_B; r; \ell_A + \ell_B' + \ell_C) + S(\ell_B; r + \ell_A; \ell_B') \leq S(\ell_B; r; \ell_A + \ell_B') + S(\ell_B; r + \ell_A; \ell_B' + \ell_C),$$

(3.75)

gives to the universal function $F_{v.N}(x)$ [20]. $S(\ell)$ is the entanglement entropy of a spin block of length $\ell$, and $S(\ell; r; \ell')$ is the entanglement entropy of two disjoint blocks of length $\ell$ and $\ell'$ at the distance $r$. We remind that strong subadditivity can be traced back to the inequalities (3.75) by exploiting the invariance of the entanglement entropy under the interchange of the subsystem with the rest (cf. Eq. (1.24)).

The first step is to rewrite Eq. (3.73) in more abstract terms, since we would like to see the consequences of strong subadditivity on $F_{v.N.}$ without any reference to the theory, and in particular to its central charge (if conformal). Thus, we recast Eq. (3.73) as follows

$$F_{v.N.}(\ell_1; r; \ell_2) = S(\ell_1) + S(\ell_2) + S(\ell_1 + \ell_2 + r) + S(r) - S(\ell_1 + r) - S(r + \ell_2) - S(\ell_1; r; \ell_2).$$

(3.76)
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This is nothing but the definition proposed in Eq. (3.62) for $F_\alpha(x)$. In the limit of large blocks in a conformal system $F(\ell_1; r; \ell_2) \to F(x)$. Eventually, by substituting Eq. (3.76) into the inequalities (3.75) we get

$$a) \quad |□||■■| \leq |◦| • ◦ \quad (3.77)$$

$$b) \quad |□□||■| \leq |◦ • | ◦ \quad ,$$

where the symbols $□$, $■$, $◦$, $•$, and $|$ are defined as follows:

1. the $n^{th}$ length is associated to the $n^{th}$ symbol, being Eq. (3.75) an inequality involving five lengths;

2. white squares $□$ and white circles $◦$ correspond to spin blocks belonging to the subsystem; black squares $■$ and black circles $•$ correspond to blocks outside of the subsystem;

3. if $A$ and $B$ are strings of squares or circles, the symbol $|$ in $A|B$ is a shorthand for the operation $A□B - A■B$ or $A ◦ B - A • B$, depending on the surrounding symbols;

4. a string of squares is the entanglement entropy of the subsystem corresponding to the configuration depicted by the string, as well as a string of circles is the universal function $F_{v,N}$ of that subsystem.

For example we have

$$□ \sim S(l_1) \quad □■ \sim S(l_1 + l_2) \quad □■□ \sim S(l_1; l_2; l_3) \quad ◦ • \sim F(l_1; l_2; l_3) . \quad (3.78)$$

The notation introduced provides a compact representation of the inequalities (3.75), expressed in terms of $F_{v,N}$, which otherwise would appear cumbersome, involving 8 terms depending on 5 variables. Notice that strong subadditivity for a single interval (1.14) can be written as $|□| \leq 0$, hence the l.h.s. of the inequalities (3.77) are lesser than or equal to 0. Now we must reduce the number of variables involved, since we would obtain inequalities for $F_{v,N}(\ell_1; r; \ell_2)$, which depends only on three variables. The first step is straightforward: in the limit in which the first length approaches 0 the symbol $|$ corresponds to the derivative with respect to the second length, hence the inequalities (3.77) are completely equivalent to

$$a) \quad □'■■ \leq ◦'| • ◦ \quad (3.79)$$

$$b) \quad □'□■ \leq ◦' • | ◦ ,$$

where we used that $f'(y) \leq 0$ implies $f(y+\delta) \leq f(y)$ for any $\delta \geq 0$. The symbols $□'$ and $◦'$ mean that we must take the derivative with respect to the corresponding length. Thus we reduced the problem to four variables. The second step is a little more involved because the symbol $|$ is surrounded by squares (circles). Actually, the symbol $|$ has the natural interpretation of moving the boundary, hence we can again restrict to infinitesimal displacements, so that we find

$$a) \quad □'■■ \leq ◦'' • ◦ - ◦' • ◦ \quad (3.80)$$

$$b) \quad □'□■ \leq ◦' • ◦ - ◦' • ◦ ,$$
3.4 $F_{v,N}(x)$: bounds from strong subadditivity

\[ a) \quad \frac{\partial^2}{\partial \ell_1^2} S(\ell_1) \leq \frac{\partial}{\partial \ell_1} \left( \frac{\partial}{\partial \ell_1} - \frac{\partial}{\partial r} \right) F(\ell_1; r; \ell_2). \]  

(3.81)

In fact we must pay attention to the order of limits when other lengths approach 0. Indeed, when the second length in (3.77) vanishes, then we cannot interpret the first symbol $|\cdot\cdot\cdot\cdot$ as a derivative, and we get

\[ c) \quad |□■■ ■■ - □ ■■■ | \leq |\cdot\cdot\cdot\cdot \circ - \circ\cdot\circ\circ\circ \]  

(3.82)

Analogously in (3.79), when the third length, or the fifth one for the second inequality, is zero we get

\[ e) \quad □'\circ - \circ'\circ \]  

(3.83)

\[ f) \quad □\circ | \leq \circ'\circ |. \]  

The inequalities $c)$ and $d)$ require a further reduction, indeed they involve four lengths. In critical systems $c)$ is trivial in the scaling limit in which the first two lengths diverge because the l.h.s. goes to $-\infty$. This means that at least one of the two lengths must be finite. If the first or the second length has the finite value $\delta$, we get

\[ c_1) \quad \delta□■■ - S(\delta) \overset{\leq}{\sim} \delta'\circ - F(\delta; \ell_1 + r; \ell_2) \]  

\[ c_2) \quad \delta□'■■ - S(\delta) \overset{\leq}{\sim} \delta(\circ'\circ - \circ\cdot\circ\circ) - F(\delta; r; \ell_2), \]  

(3.85)

where we called the remaining lengths $\ell_1$, $r$, and $\ell_2$. The inequalities are trivial because $S(\delta)$ is the only finite quantity in the scaling limit $\ell_1 \sim r \sim \ell_2 \to \infty$, hence we get simply the positivity of the entanglement entropy of a single block. The inequality $d)$ is more interesting. If the second and the fourth lengths are different from 0 the symbol $|$ can be interpreted as an infinitesimal displacement of the boundary

\[ d) \quad |□ | \leq \circ\cdot\circ' - \circ\circ\circ, \]  

(3.86)

i.e.

\[ d) \quad \frac{\partial}{\partial r} [S(\ell_1 + r) - S(r)] \leq \left( \frac{\partial}{\partial \ell_2} - \frac{\partial}{\partial r} \right) F(\ell_1; r; \ell_2). \]  

(3.87)

If the second length is zero the inequality is trivial because the l.h.s. diverges for any interesting value of the r.h.s., as it happens for the inequality $c)$. If instead the fourth length is zero we get

\[ d_1) \quad \nabla | \leq \circ\cdot\circ, \]  

(3.88)
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Figure 3.10: Strong subadditivity - TTN (tree tensor network) data for the von Neumann entropy in the XXZ chain, whose Hamiltonian is given by $H_{XXZ} = 4H_{XX}^{b=0} + \Delta \sum_l \sigma_l^x \sigma_{l+1}^x$, for various values of $\Delta$ in the interval $\Delta \in [-0.3, 1]$. Different symbols mean different values of $\Delta$, different colors stand for different $\ell$ and lattice sizes (Figure 22 of Ref. [74]). We added the region that strong subadditivity allows for $\Delta = -0.3$ (we extracted the estimate of $F_{V,N}(1/2)$ from the data).

that is

$$d_1) \quad S(\ell_1 + r + \ell_2) + S(r) - S(\ell_1 + r) - S(r + \ell_2) \leq F(\ell_1; r; \ell_2). \quad (3.89)$$

Now we consider conformal systems. In every inequality $a), b), d), d_1), e),$ and $f)$ the universal function $F_{v,N}$ is put in relation with quantities proportional to the central charge $c$, since the entanglement entropy of a single block is proportional to $c$. Thus, it is natural to write the inequalities for the quantity $\tilde{F}_{v,N} = 3F_{v,N}/c$. By expressing all in terms of the variables $x, \ell_1,$ and $\ell_2$ and using that $F = F(x)$ we obtain

$$a) \quad \frac{\partial}{\partial x}(1-x) \frac{\partial}{\partial x} \tilde{F}(x) \geq -\frac{1}{x^2}$$

$$b) \quad \frac{\partial}{\partial x}x(1-x) \frac{\partial}{\partial x} \tilde{F}(x) \geq -1$$

$$d), f) \quad \frac{\partial}{\partial x} \tilde{F}(x) \geq -\frac{1}{1-x}$$

$$d_1) \quad \tilde{F}(x) \geq \log(1-x)$$

$$e) \quad \frac{\partial}{\partial x} \tilde{F}(x) \leq \frac{1}{x}.$$ 

(3.90)

Because we are in the thermodynamic limit, we must impose the symmetry $F(x) = F(1-x)$ by hand. Otherwise the relations (3.79) are not sufficient to characterize completely strong
subadditivity. Eventually, from the inequalities (3.90) we get the bounds

\[
\max \left[ \log(1-x), \frac{1}{2} \log[4x(1-x)] \right] \leq \tilde{F}(x) \leq \frac{1}{2}\log[4x(1-x)] \quad x < 1/2. \quad (3.91)
\]

In particular, \( \tilde{F}(1/2) \geq -\log 2 \). The conditions (3.91) do not seem very strong. The upper bound increases as \( x \) decreases, and the lower bound \( \log(1-x) \) is negative; instead, the approximate data obtained in Ref. [67,74] by tree tensor network algorithms, in CFTs with \( c = \frac{1}{2} \) and \( c = 1 \), suggest that \( F_{v,N} \) could be always a positive concave function of \( x \). Thus, we face with the puzzle of the divergence between the natural surmise of concavity and positivity, on the basis of numerical analyses, and the apparently too weak bounds given by strong subadditivity.

In the next section we provide numerical evidence that the universal functions can be indeed negative. Anyway, \( \tilde{F}(1/2) + \frac{1}{2}\log[4x(1-x)] \) is a weak but non-trivial lower bound. In Figure 3.10 the data obtained in Ref. [74] are compared with the bounds given by strong subadditivity.

3.5 Remarks

**Symmetry** \( x \leftrightarrow 1-x \). In this paragraph we investigate the symmetry under interchanging the subsystem with the rest. The transformation acts on the block entanglement entropies as follows:

\[
(A_1B_1A_2 \rightarrow B_1A_2B_2) \Rightarrow \begin{cases}
S_{t_1} \rightarrow S_{t_1+r+\ell_2} \\
S_r \rightarrow S_{t_1} \\
S_{\ell_2} \rightarrow S_r \\
S_{t_1+r+\ell_2} \rightarrow S_{\ell_2}
\end{cases}
\quad (3.92)
\]

where we used the state’s purity in order to express the entanglement entropies in terms of the lengths of \( A_1, B_1, \) and \( A_2 \). The diagonalization of the transformation (3.92) is straightforward

\[
(1) : \begin{cases}
S_{t_1} + S_r + S_{\ell_2} + S_{t_1+r+\ell_2} \\
S_{t_1+r} + S_{r+\ell_2}
\end{cases} \\
(-1) : \begin{cases}
S_{t_1} - S_r + S_{\ell_2} - S_{t_1+r+\ell_2} \\
S_{t_1+r} - S_{r+\ell_2}
\end{cases} \\
(\pm i) : S_{t_1} - S_{\ell_2} \pm i(S_{t_1+r+\ell_2} - S_r)
\quad (3.93)
\]

where the first number is the eigenvalue. Any invariant is a function of the eigenvectors corresponding to the eigenvalue 1. We would define \( x \) in such a way that the transformation would act as a reflection about \( \frac{1}{2} \), i.e. \( x \rightarrow 1-x \). In addition we ask for \( x \) to be the four point ratio in the scaling limit of a conformal system. Notice that

\[
\log \frac{1-x}{x} \rightarrow -\log \frac{1-x}{x} \quad (3.94)
\]
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and hence \( \log \frac{1-x}{x} \) belongs to the eigenspace corresponding to the eigenvalue \(-1\). We see immediately that \( x \) can be defined as

\[
x \equiv \frac{1}{1 + \exp \left( \frac{3}{c} \left( S_{\ell_2+r+t_2} + S_r - S_{\ell_1} - S_{\ell_2} \right) \right)},
\]

where we used that

\[
S_\ell \sim \frac{c}{3} \log \ell.
\]

However, this is not the end of the story: \( F_\alpha \) is a function of \( x \) only in the scaling limit. Otherwise it depends on other lengths too. Notice that the eigenfunctions corresponding to the eigenvalue 1 of the symmetry transformation (3.92), once \( x \) is fixed, are dependent (at least asymptotically)

\[
S_{\ell_1} + S_r + S_{\ell_2} + S_{\ell_1+r+t_2} \sim 2(S_{\ell_1+r} + S_{r+t_2}) + \frac{c}{3} \log[(1-x)x]
\]

hence we can not take both of them together as further independent variables. This has the unpleasant consequence that the corrections to the scaling do not preserve the symmetry \( x \leftrightarrow 1-x \). Indeed one of the other two variables can not be invariant. We choose the variables \( \lambda \equiv \exp \left[ \frac{3}{2c} (S_{\ell_1+r} + S_{\ell_2+r}) \right] \) and \( \ell_1 \). In fact, the function \( F^{\text{lat}} \) is invariant under the transformation (3.92), hence we can write the correction to the scaling as follows:

\[
F^{\text{lat}} - F^{\text{CFT}} \approx e^{-\frac{3}{16}S_{\ell_1}} + e^{-\frac{3}{16}S_{\ell_2}} h_\lambda(x) + e^{-\frac{3}{16}S_{\ell_1+r+t_2}} + e^{-\frac{3}{16}S_r} h_\lambda(1-x) + \frac{g_\lambda(x)}{\lambda^\delta},
\]

where we assumed that the functions \( h_\lambda \) and \( g_\lambda \) have no further dependences on \( \ell_1 \) (for example, even-odd oscillations). By considering blocks of equal lengths, the symmetry implies

\[
F^{\text{lat}}(x; \lambda) - F^{\text{CFT}}(x) \approx \frac{1}{\lambda^\delta} \left[ h(x) + \frac{(1-\sqrt{x})^\delta + (1+\sqrt{x})^\delta}{2(1-x)^\frac{\delta}{2}} h(1-x) + g((1-2x)^2) \right].
\]

In fact, the functional form is not constraining at all. Observe that the symmetry is recovered as the critical exponent \( \delta \), which controls the correction to the scaling, approaches 0. We expect a larger asymmetry for models with a larger value of \( \delta \). And the first correction to \( F_\alpha \) should be more symmetric for large values of \( \alpha \) (remind \( \delta \sim \frac{2y}{c} \)). Because

\[
\ell \approx \frac{\lambda}{\sqrt{x}}
\]

we see that the correction at fixed block’s length \( \ell \) can be obtained by multiplying by \( x^{\frac{\delta}{2}} \) the correction at \( \lambda \) fixed. By analyzing the Ising chain, the XX model, and by considering the Monte Carlo data obtained in Ref. [74] for the corrections to the scaling in some models with central charge \( c = 1 \) (Figure 3.11) we see that the correction at \( \lambda \) fixed could really remain different from 0 as \( x \to 0 \) (observe in particular the data relative to the XX model). Thus we expect \( \tilde{f}_\alpha(0) \neq 0 \), where

\[
F^{\text{lat}}_\alpha(x, \ell) \sim F_\alpha(x) + \frac{\tilde{f}_\alpha(x)x^{\frac{\delta}{2}}}{\ell^\delta} + \ldots.
\]
so that \( f_\alpha(x) \sim x^{\frac{\delta}{2}} \) (cf. Eq. (3.56)) for sufficiently small \( x \). In any model in which this is true, the exponent governing the small \( x \) behavior of the correction to the scaling of \( F_\alpha \) at \( \ell \) fixed is half of the scaling dimension \( \delta \) of the operator responsible for the correction \( \sim \ell^{-\delta} \).

**On the positivity of \( F_\alpha(x) \).** Here we show an example in which \( F_2 \) displays a counterintuitive behavior, suggesting the possibility of some unusual feature (such as non concavity and/or positivity) for \( F_{v,N} \). We consider the excited state of the XX chain that is the ground state of the Hamiltonian

\[
H_{XX3} = \frac{1}{4} \sum_l \left( \sigma^x_l \sigma^x_{l+1} \sigma^z_{l+2} \sigma^z_{l+3} + \sigma^y_l \sigma^x_{l+1} \sigma^x_{l+2} \sigma^z_{l+3} \right).
\]

This can be diagonalized in the same way as we diagonalized the XX Hamiltonian (2.36), obtaining the dispersion relation

\[
\varepsilon_{XX3}(\varphi) = |\cos(3\varphi)|,
\]

which corresponds to a CFT with central charge \( c = 3 \) (there are 6 chiral modes). In fact, the continuum limit of the corresponding fermionic Hamiltonian is the tensor product of three free bosons, and one could argue erroneously that the universal functions should be given by \( F_{XX}^3(x) \). This is wrong for the same reason for which the universal function in the fermionic representation is different from that in the spin representation. Indeed the fermionic Hamiltonian is given by

\[
H_{XX3}^{fr} = -\frac{1}{2} \sum_l (c^+_l c_{l+3} + h.c.) = -\frac{1}{2} \sum_l (a^+_l a_{l+1} + b^+_l b_{l+1} + d^+_l d_{l+1})
\]
Figure 3.12: $F_2$ for a model with central charge equal to 3. The universal function $F_2$ for the ground state of the conformal system with central charge $c = 3$, whose Hamiltonian is given by Eq. (3.102) (in fact, it is an eigenstate of the XX Hamiltonian). The universal function is obviously lesser than 1. In the second graph we kept $\ell + r$ as fixed, obtaining an almost symmetric function: the empty symbols are the mirror image about $x = \frac{1}{2}$ of the full symbols. The curve is the prediction (3.107). This is the first numerical evidence of the possibility to have $F_\alpha(x) < 1$. 
where we defined the fermions $a_l \equiv c_{3l}$, $b_l \equiv c_{3l+1}$, and $d_l \equiv c_{3l+2}$. The Hamiltonian restricted to the set of sites congruent modulo 3 is independent of the other fermions. This is not true anymore for the Hamiltonian \(3.102\), in which the three commuting operators, corresponding to the fermionic sectors, are not defined in separate spatial regions. Eventually we get

\[
\text{Tr} \rho^2 = \left\{ \Gamma_2 \right\}^3 + \left\{ \Gamma_1, \Gamma_2 \right\}^3 + \langle a_B^+ \rangle^6 \left\{ \Gamma_3 \right\}^3 - \left\{ \Gamma_3, \Gamma_4 \right\}^3,
\]

(3.105)

where the correlation matrices are the XX ones corresponding to the subsystem in which any length is divided by 3. This can be understood easily, indeed each fermionic RDM in Eq. (3.12) factorizes in the three independent fermionic spaces consisting of the sites congruent modulo 3. Thus, Eq. (3.105) follows immediately. The universal function $F_2(x)$ can be calculated analytically by exploiting the relations \[20\]

\[
\left\{ \Gamma_2, \Gamma_1 \right\} \sim \sqrt{1-x}\{\Gamma_1^2\}
\]

\[
\langle a_B^+ \rangle^2 \{\Gamma_3^2\} \sim \sqrt{x}\{\Gamma_1^2\}
\]

\[
\langle a_B^+ \rangle^2 \{\Gamma_3, \Gamma_4\} \sim 0,
\]

(3.106)

satisfied by the correlation matrices of the XX model in the scaling limit. Finally, using that $\Gamma_1$ is the correlation matrix in the fermionic representation ($F_{fer}^2(x) = 1$) we get \[20\]

\[
F_2(x) = 1 + x^\frac{3}{2} + (1-x)^\frac{3}{2}.
\]

(3.107)

In Fig. 3.12 the universal function $F_2(x)$ is shown for various values of $\ell_1 = \ell_2 = \ell$ and many distances. In the second graph the same function is plotted fixing $\ell + r$. Observe that the symmetry $x \leftrightarrow 1-x$ is almost restored. This is the first example of a model in which $F_2(x) < 1$. The function approaches 1 linearly as $x \to 0$. This is not in contrast with the small $x$ expansion of Ref. \[27\]

\[
F_2(x) \sim 1 + N \left( \frac{x}{16} \right)^\alpha + O(x^{2\alpha}) + O(x):
\]

(3.108)

in our model $\alpha = \frac{3}{4} > 1$, so that the linear term is leading

\[
F_2(x) \sim 1 - \frac{3}{4}x + \frac{1}{2}x^{\frac{3}{2}}.
\]

(3.109)

Incidentally, we find that the number of inequivalent correlation functions giving the same contribution $N$ (see Ref. \[24\]) is equal to 32. The coefficient of the linear term is in agreement with the observation in Ref. \[27\] (cf. Eq. 70 and 71 there) that a simple $O(x)$ contribution comes from the denominator of Eq. (3.57), for the free boson compactified on a circle, or Eq. (3.63), for the Ising model, and which is expected to have the general form

\[
-\frac{c}{6} (n - \frac{1}{n}) x.
\]

(3.110)

In our case $c = 3$, it gives the correction $-\frac{3}{2}x$ in Eq. (3.109). The facts that $F_2(x)$ is convex and it approaches 0 linearly suggest that the universal function $F_{v,N}$ could be negative. Indeed,
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the scaling dimension of the same operator determines the exponent of the small $x$ behavior for both $F_{v,N}$ and $F_\alpha$. Because $\alpha = \frac{3}{2}$ we expect

$$F_{v,N}(x) \sim kx + \frac{3\pi}{8}x^{\frac{3}{2}} + O(x^2),$$  \hspace{1cm} (3.111)

where we exploited the small $x$ expansion (3.74) to predict the coefficient of $x^{3/2}$. $k$ can be inferred by analytically continuing the correction (3.110), i.e.

$$k = -\frac{c}{3} = -1$$  \hspace{1cm} (3.112)

If the small-$x$ expansion discussed above can be applied to our system, we have found the first case in which $F_{v,N}$ is negative for sufficiently small $x$. On the other hand $|F_{v,N}|$ could be again a concave function of $x$. In fact, these are very preliminary results and only the analysis of the small-$x$ behavior in several theories could help understanding the peculiar features of the universal function $F_{v,N}$.

The next section is a complement to Sec. 3.1 in which the formalism introduced to study the Renyi entropies of two disjoint blocks in the XY model is generalized to many disjoint blocks.

3.6 Many disjoint blocks

The fermionic density matrix equivalent to the spin RDM of more than 2 disjoint blocks can be obtained once again from Eq. (3.4). The only complication is that the decomposition

$$\prod_{l \in S} a^z_l = \prod_{l \in \overline{B}_l \subset \Omega} \sigma^z_l \prod_{l \in \Omega \setminus \Omega} \sigma^z_l \quad S \subset \Omega$$  \hspace{1cm} (3.113)

defines more operators outside of the subsystem in the fermionic representation. If $n_A$ is the number of disjoint blocks, the JW strings $a^z$ responsible for the inequivalence of the spin and fermionic representations are products of the $\sigma_z$ strings inside of the holes $B_l$

$$a^z_{\{\sigma\}_l} \equiv \prod_{l=1}^{n_A-1} \frac{1 + \sigma_l}{2} a^z_{B_l} + \frac{1 - \sigma_l}{2} I \quad \sigma_l \in \{-1,1\}.$$  \hspace{1cm} (3.114)

The string $a^z_{\{\sigma\}_l}$ multiplies the operators in which the parity of the total number of fermions in the blocks that follow $A_l$ is $\sigma_l$, i.e. the parity of the fermions in $A_l$ is equal to $\prod_{j=l-1}^{n_A-1} \sigma_j$. The $2^{n_A-1}$ strings $a^z_{\{\sigma\}_l}$ commute with the density matrix. Their eigenvalues, namely $\pm 1$, are determined by the eigenvalues of the strings $a^z_{B_l}$. The configuration $\sigma_l = -1$ for any $l$ corresponds to the identity. Thus we find $2^{n_A-1}$ equivalent fermionic representations characterized by the eigenvalues $\tau_l$ of the strings $a^z_{B_l}$

$$\rho_A = \sum_{\{\tau\}} \left( \prod_{l=1}^{n_A-1} \frac{1 + \tau_l a^z_{B_l}}{2} \right) \rho^{(\tau)}_A,$$  \hspace{1cm} (3.115)
with
\[
\rho_A^{(\gamma)} = \frac{1}{2^n_A} \sum_{\{\sigma\}} \langle a_{\{\sigma\} B} \rangle^n_A \prod_{l=1}^{n_A-1} \frac{1+\epsilon_l}{\epsilon_l} \sum_{\{\sigma'\}} \epsilon([\sigma']) [\sigma] a_{\{\sigma'\} A} \rho_A^{(a_{\{\sigma'\} B})} a_{\{\sigma'\} A}. \tag{3.116}
\]

The product \(\prod_{l=1}^{n_A-1} \frac{1+\epsilon_l}{\epsilon_l}\) is the eigenvalue of \(a_{\{\sigma\} B}^{*}\), and the string \(a_{\{\sigma\} A}^{*}\) is defined as
\[
a_{\{\sigma\} A}^{*} = \prod_{l=1}^{n_A-1} \frac{1+\epsilon_l}{2} a_{A_{\gamma+1}}^{*} + \frac{1-\epsilon_l}{2} \sigma_l \quad \sigma_l \in \{-1, 1\}. \tag{3.117}
\]

The sign \(\epsilon([\sigma']) [\sigma]\) is the parity of the block \(a_{\{\sigma'\} A}^{*}\) corresponding to the configuration \(a_{\{\sigma\} B}^{*}\), that is to say
\[
\epsilon([\sigma']) [\sigma] = \prod_{l, \text{s.t. } \sigma_l'=1}^{n_A-1} \prod_{j=1}^{\sigma_j} \prod_{i=1}^{\sigma'_j} \sigma_j = \prod_{l=1}^{n_A-1} \langle \sigma_j \rangle_{\sum_{l'=1}^{n_A-1} 1+\epsilon_l'} \frac{1+\epsilon_l'}{2}. \tag{3.118}
\]

The density matrices \(\rho^{(a_{\{\sigma'\} B})} = a_{\{\sigma'\} A}^{*} \rho_A^{(a_{\{\sigma'\} B})} a_{\{\sigma'\} A}\) are Gaussian. The explicit form of the correlation matrices \(\Gamma^{(\sigma')}\) is a simple generalization of the double block case
\[
\Gamma^{(\sigma')} = \left( \prod_{l, \sigma_l'=1}^{n_A} P_{l+1} \otimes I_2 \right) \Gamma_{A_{\gamma} \cup (\cup_{l, \sigma_l'=1} B_l)} / \Gamma_{\cup_{l, \sigma_l'=1} B_l} \left( \prod_{l, \sigma_l'=1}^{n_A} P_{l+1} \otimes I_2 \right) \tag{3.119}
\]
where \(P_l\) is the diagonal matrix with any diagonal element equal to 1, except for those corresponding to the block \(A_l\), which are equal to \(-1\). We indicated with \(A_{11} / A_{22}\) the Schur complement \(A_{11} - A_{12} A_{22}^{-1} A_{21}\), where \(A\) is the \(2 \times 2\) block matrix made of the blocks \(A_{ij}\). Notice that \(\langle a_{\{\sigma\} B}^{*} \rangle = i \sum_{l=1}^{n_A-1} \frac{1+\epsilon_l}{2} \text{Tr}(\Gamma_{\cup_{l, \sigma_l'=1} B_l})\). Rényi entropies can be computed in the same way as when the subsystem consists of just two disjoint blocks. But many more terms contribute. And when the number of blocks is comparable with the chain size we expect an extensive behavior of Rényi entropies, as observed in [18], which is reminiscent of the huge number of fermionic RDMs needed to represent the spin RDM.

Here we consider the case \(n_A = 3\), for instance. The spin RDM reads as
\[
\rho_{A_1 \cup A_2 \cup A_3} = \frac{1}{2^{n_1+2q+T}} \sum_{e_1 e_2 e_3} \langle O_1 O_2 O_3 \rangle O_3^1 O_2^1 O_1^1 + a_{B_1}^{\gamma} \sum_{e_1 e_3 e_3} \langle a_{B_1}^{\gamma} O_1 O_2 O_3 \rangle O_3^1 O_2^1 O_1^1 + a_{B_2}^{\gamma} \sum_{e_2 e_2 e_3} \langle a_{B_2}^{\gamma} O_1 O_2 O_3 \rangle O_3^1 O_2^1 O_1^1, \tag{3.120}
\]
where the sums are intended over all possible products of Majorana fermions belonging to each interval and \(c_i/o_i\) (even/odd) refers to the parity of the number of Majorana operators in the block \(A_i\). We choose the fermionic representation in which the eigenvalues \(\tau_i\) of \(a_{B_i}^{\gamma}\) are all
equal to 1 (cf. Eq. (3.115)). The RDM is sum of 16 Gaussian RDMs:

\[
\rho_{A_1 \cup A_2 \cup A_3}^{++} = \frac{\rho_{er}^{A} + a_{A_2}^{z}\rho_{er}^{A} a_{A_2}^{z} + a_{A_2}^{\dagger} a_{A_2}^{z}\rho_{er}^{A} a_{A_2}^{\dagger} a_{A_2}^{z}}{4} + \frac{\langle a_{B_1}^{z} \rangle^{(a_{B_1}^{z})} - a_{A_2}^{z}\rho_{er}^{A} a_{A_2}^{z}}{4} + \frac{\langle a_{B_2}^{z} \rangle^{(a_{B_2}^{z})} - a_{A_2}^{z}\rho_{er}^{A} a_{A_2}^{z}}{4} + \frac{\langle a_{B_1}^{z}, a_{B_2}^{z} \rangle^{(a_{B_1}^{z}, a_{B_2}^{z})} - a_{A_2}^{z}\rho_{er}^{A} a_{A_2}^{z}}{4} + \frac{\langle a_{B_1}^{z}, a_{B_2}^{z} \rangle^{(a_{B_1}^{z}, a_{B_2}^{z})} - a_{A_2}^{z}\rho_{er}^{A} a_{A_2}^{z}}{4} + \frac{\langle a_{B_1}^{z}, a_{B_2}^{z} \rangle^{(a_{B_1}^{z}, a_{B_2}^{z})} - a_{A_2}^{z}\rho_{er}^{A} a_{A_2}^{z}}{4}.
\]

(3.121)

In general the RDM of \( n_A \) disjoint blocks is equivalent to a fermionic operator, sum of \( 4^{n_A-1} \)
Gaussian RDMs. We also report the second moment of the density matrix

\[
\text{Tr} \rho_{A_1 \cup A_2 \cup A_3}^{\rho} = \frac{\{\Gamma_1, \Gamma_1\} + \{\Gamma_1, \Gamma_2\} + \{\Gamma_1, \Gamma_3\} + \{\Gamma_1, \Gamma_4\}}{4} + \frac{|\det \Gamma_{B_1}| \{\Gamma_1^{(1)}, \Gamma_1^{(1)}\} - \{\Gamma_1^{(1)}, \Gamma_1^{(1)}\}}{4} + \frac{|\det \Gamma_{B_2}| \{\Gamma_1^{(2)}, \Gamma_1^{(2)}\} - \{\Gamma_1^{(2)}, \Gamma_1^{(2)}\}}{4} + \frac{|\det \Gamma_{B_2} \Gamma_{B_1}| \{\Gamma_1^{(12)}, \Gamma_1^{(12)}\} - \{\Gamma_1^{(12)}, \Gamma_1^{(12)}\}}{4} + \frac{|\det \Gamma_{B_2} \Gamma_{B_1}| \{\Gamma_1^{(12)}, \Gamma_1^{(12)}\} - \{\Gamma_1^{(12)}, \Gamma_1^{(12)}\}}{4}.
\]

(3.122)

where \( \Gamma_1 \) is the fermionic RDM, \( \Gamma_{2(3)} \equiv (P_{2(3)} \otimes I) \Gamma_1 (P_{2(3)} \otimes I), \Gamma_{23} \equiv (P_{2} P_{3} \otimes I) \Gamma_1 (P_{2} P_{3} \otimes I), \)
and the superscripts mean

\[
\Gamma^{(1)} \equiv \frac{\Gamma_{A \cup B_1} / \Gamma_{B_1}}{\Gamma_{A \cup B_1} / \Gamma_{B_1}}, \quad \Gamma^{(2)} \equiv \frac{\Gamma_{A \cup B_2} / \Gamma_{B_2}}{\Gamma_{A \cup B_2} / \Gamma_{B_2}}, \quad \Gamma^{(12)} \equiv \frac{\Gamma_{A \cup B_1 \cup B_2} / \Gamma_{B_1 \cup B_2}}{\Gamma_{A \cup B_1 \cup B_2} / \Gamma_{B_1 \cup B_2}}.
\]

(3.123)

In practice this term, that is to say the Rényi entropy \( S_2 \), is the only one computable efficiently
with the formalism developed in Ref. [9] and described in this chapter, since the number of
terms grows rapidly. In fact this method has polynomial complexity in the subsystem’s lengths
but it requires exponential numerical efforts in terms of the number of blocks and of the Rényi
index.

In conclusion, our formalism has been useful to compute the first integral Rényi entropies
of large subsystems consisting of two disjoint blocks, and could be used to investigate \( S_2 \), and
\( S_3 \) at the most, of three disjoint blocks.

A major problem remains still open. We are unable to find all the eigenvalues of the
reduced density matrix of disjoint subsystems and so the Rényi entropies for non-integer \( \alpha \) and
in particular for \( \alpha = 1 \) that would give the widely studied von Neumann entropy. The same
problem is also present in conformal calculations. It is possible to obtain \( \text{Tr} \rho_{A}^{\alpha} \) only for \( \alpha \) integer
[14,27] and the analytic continuation of the result to general complex values remains a big open
problem.
3.6 Many disjoint blocks

Notice also that the contribution of the Jordan-Wigner string also affects the entanglement entropy of a single interval in a system with one or more boundaries, if the block $A$ does not include the boundary.

Finally, we mention that the same structure characterized by the sum of a finite number of Gaussian RDMs is found when taking the partial transpose of a fermionic RDM [20], which is the main ingredient for the calculation of the entanglement between two blocks $A_1$ and $A_2$, or of a block at finite temperature, measured by negativity (see e.g. [31,32]).

In this chapter we analyzed the entanglement entropies of disjoint subsystems. The behavior of the integer Rényi entropies is only known for a few conformal systems, and we reported the CFT results. Many difficulties arise in obtaining numerical data. However, we developed a formalism which solves partially these problems and allow to get the first integer Rényi entropies in models with a free-fermion representation. We checked the CFT predictions and we faced with the corrections to the scaling, which become larger and larger, as the Rényi index $\alpha$ increases. In particular we studied the universal part of the corrections, which has been recently understood in the framework of CFT. In the next chapter we will examine in more details the corrections to the scaling. We will use the XX chain as testing ground for the CFT results, focusing on the effects of boundary conditions on the corrections to the scaling.
3. ENTANGLEMENT ENTROPIES OF DISJOINT SUBSYSTEMS
4. Beyond the asymptotic behavior

In the previous chapters we investigated the leading behavior of entanglement entropies in one-dimensional systems. The part of the entropies that diverges as the logarithm of the subsystem’s length, in a conformal system, is proportional to the central charge of the CFT. We also analyzed disjoint subsystems and we realized that further universal features can be extracted from the non-divergent part, namely the universal functions \( F_\alpha(x) \). For these reasons a scaling analysis of \( S_\alpha \) is increasingly used in numerical studies of quantum phase transitions in one-dimensional systems. In such applications \( S_\alpha(\ell) \) is computed numerically and the large-\( \ell \) behavior is then fitted to the CFT prediction

\[
S_\alpha(\ell) \approx \begin{cases} 
\frac{c}{6} \left( 1 + \frac{\alpha}{2} \right) \log \ell + c'_\alpha & \text{PBC} \\
\frac{c}{12} \left( 1 + \frac{\alpha}{2} \right) \log(2\ell) + \frac{1}{2} c'_\alpha + \log g & \text{OBC}
\end{cases}
\] (4.1)

where \( c'_\alpha \) are non-universal additive constants, \( g \) and \( \log g \) is the boundary entropy, first discussed by Affleck and Ludwig \cite{75}. As in the previous chapters, PBC stands for periodic boundary conditions and OBC for open boundary conditions. In particular, for the XX model with OBC (which we are going to analyze), we have \( g = 1 \) \cite{75}. As already mentioned considering the entanglement entropy of disjoint blocks, the asymptotic result is sometimes obscured by large, and often oscillatory, corrections to the scaling \cite{76,77}. These corrections are considered universal, and encode information about the underlying CFT. More precisely, they give access to the scaling dimensions of some of the most relevant operators \cite{70}. For a Luttinger liquid, the proposed scaling form of \( S_\alpha \) is \cite{71}

\[
S_\alpha = S_\alpha^{CFT} + f_\alpha \cos(2k_F \ell) \ell^{-2K/\alpha},
\] (4.2)

where \( K \) is the scaling dimension of a relevant operator (in general the oscillating factor can be different from \( \cos(2k_F \ell) \) or even be absent, as it happens for the Ising model). The constant \( f_\alpha \) is a non-universal quantity. It has been determined exactly for XX and Ising models in Refs. \cite{71,78}. Actually, because of strong subadditivity (cf. Eq. (1.14)), oscillations are absent in

\footnote{Notice that \( c'_\alpha \) is equal to \( \frac{\log c_\alpha}{\alpha^{2}} \), where \( c_\alpha \) is defined in Eq. (\ref{eq:3.1})}
the entanglement entropy of periodic systems: \( f_1 \) is equal to 0. In addition, on the basis of universality and directly by CFT, it has been argued that in the case of OBC, the exponent governing the corrections is half of the PBC one (i.e. \( K/\alpha \) replaces \( 2K/\alpha \) in Eq. (1.2)). It is important to mention that, with OBC, oscillatory corrections are also present for \( \alpha \to 1 \), indeed strong subadditivity does not forbid oscillations (cf. Eq. (1.29)).

A precise characterization of the subleading terms in \( S_\alpha(\ell) \) is desirable for two reasons. First, the knowledge of their structure will be helpful when using Eqs. (4.1) to extract the central charge from numerical computations of \( S_\alpha(\ell) \). Second, the subleading terms can be used to infer the scaling dimension of certain operators in the CFT characterizing the quantum critical point, in the same way as in analysing disjoint subsystems in the critical Ising model we recognised the existence of an operator with scaling dimension \( \frac{1}{2} \).

In this chapter we compute analytically the entanglement entropies in the XX chain at order \( o(\ell^{-1}) \), both with periodic and open boundary conditions, as done in Refs. [11 78]. From a purely mathematical point of view the study of corrections to the scaling in the XX chain leads to the problem of calculating the leading and subleading behavior of the determinants of matrices that, in mathematical literature, are known as Toeplitz (PBC) and Toeplitz plus Hankel (OBC). Toeplitz (Hankel) are structured matrices that depend only on the difference (sum) between row and column indices. Toeplitz matrices have a very long history, culminating with the Fisher-Hartwig (FH) conjecture [79]. This conjecture has been proved (in some particular cases) only many years after its formulation by Basor [80]. The interest in the corrections to this formula leaded to a generalization known as generalized FH conjecture [81] that has not yet been proved. This formula has been fundamental to provide the corrections to the scaling for the entanglement entropy in systems with PBC. When moving from PBC to OBC, we move from Toeplitz matrices to Toeplitz plus Hankel ones, that is a brand new field of mathematics. The formula generalizing FH has been proved very recently [61], and in Ref. [11] we conjectured a generalized FH formula for the particular Toeplitz plus Hankel matrices that arise considering the XX chain with OBC. Eventually, putting together the ingredients of the generalized FH and the recent results for Toeplitz plus Hankel, we determined analytically the corrections to the scaling of the entanglement entropy for OBC.

Here we report the asymptotic expression of the entanglement entropies of a block in the periodic XX chain, up to \( O(\ell^{-2/\alpha}) \) [1178]

\[
S_{\alpha}^{PBC}(\ell) = \frac{1}{6} \left( 1 + \frac{1}{\alpha} \right) \ln |\ell| \sin k_F| + E_\alpha + \frac{2 \cos [2k_F \ell]}{1 - \alpha} \left\{ [2|\ell| \sin k_F]|^{-1/\alpha} \frac{\Gamma \left( \frac{1}{2} + \frac{1}{2\alpha} \right)}{\Gamma \left( \frac{1}{2} - \frac{1}{2\alpha} \right)} \right\}^2
\]

\[
S_{v.N.}^{PBC} = \frac{1}{3} \log |\ell| \sin k_F| + E_1 - \frac{1}{12\ell^2} \left( \frac{1}{5} \cot^2 k_F \right).
\]

Notice that the von Neumann entropy cannot be obtained from the right limit of the first equation as \( \alpha \) approaches 1, indeed the subleading corrections to the Renyi entropies must be taken into account. Observe also that oscillations are absent in \( S_{v.N.} \), according to the analysis in Chapter 1, strong subadditivity is not compatible with oscillations.
Instead, the entanglement entropies of a block staring from the boundary of the semi-infinite XX chain up to $O(\ell^{1/\alpha})$ are given by

$$S_{OBC}^{\alpha}(\ell) = \frac{1}{12} \left(1 + \frac{1}{\alpha}\right) \ln \left[2(2\ell + 1)\sin k_F\right] + \frac{E_\alpha}{2}$$

$$+ \frac{2\sin[2k_F(\ell + \frac{1}{2})]}{1 - \alpha} |2(2\ell + 1)\sin k_F|^{-1/\alpha} \frac{\Gamma(\frac{1}{2} + \frac{1}{\alpha})}{\Gamma(\frac{1}{2} - \frac{1}{\alpha})}$$

$$S_{v.N.}^{OBC} = \frac{1}{6} \log \left[2(2\ell + 1)\sin k_F\right] + \frac{E_1}{2} - \frac{\sin[k_F(2\ell + 1)]}{2(2\ell + 1)\sin k_F}.$$  

Notice that away from half-filling $(k_F = \pi/2)$, the oscillations have different forms compared to the PBC case (4.3). While these formulae are correct only to order $o(\ell^{1/\alpha})$ for PBC and to order $o(\ell^{-1/\alpha})$ for OBC, in the following we will present the full expansion up to the order $o(\ell^{-1})$, for any finite value of $\alpha$. In the case of $\alpha \to \infty$, the corrections become logarithmic and are also exactly calculated. Most of the similarities and differences between Eq. (4.3) and Eq. (4.4) can be understood in the framework of CFT: in the following paragraph we review the basic CFT results that underly these general properties.

**OBC vs PBC: a CFT survey.** The entanglement entropies $S_\alpha$ of a finite interval $A \equiv [0, \ell]$ in a semi-infinite system $[0, \infty)$ can be obtained by exploiting the path integral representation (1.39) of the RDM’s moments. In particular, one can use the mapping of the $\alpha$-sheeted Riemann surface $R_\alpha[A]$, where the path integral (1.39) is defined, to the unit disk $|z| = 1$ [34]. By calling $x$ the spatial variable and $\tau$ the imaginary time, the uniformising transformation is $z = \left(\frac{\tau + ix}{2\ell + i\tau}\right)^{1/\alpha}$, where $w = \tau + ix$. In the disk the expectation value of the stress tensor is zero, by rotational invariance, so that (cf. the first equality of Eq. (1.52) and the Ward identity (1.53)) we get

$$\langle T \rangle_{R_\alpha[A]} = \frac{c(1 - \alpha^{-2})}{24} \frac{(2\ell)^2}{(w - i\ell)^2(w + i\ell)^2}.$$  

Using the same procedure as in absence of the boundary (cf. the first equality of Eq. (1.52) and the Ward identity (1.53)) we get

$$\text{Tr} \rho^\alpha \sim \tilde{c}_\alpha(2\ell/a)^{\frac{1}{\alpha} - 1/\alpha}.$$  

and hence

$$S_\alpha = \frac{c}{12} \frac{1 + \alpha}{\alpha} \log(2\ell) + \text{const.}.$$  

By looking more carefully at the procedure sketched above we see that the conformal transformation is mapping the semi-infinite system into an infinite one, by joining the former with its mirror image through the boundary. This picture can be used to understand the origin of the factor 2 multiplying $\ell$ and of the other factor 2 dividing the entanglement entropies in the semi-infinite system, in contrast with the expressions in the infinite one: the subsystem doubles joining to its mirror image, while the overall $\frac{1}{2}$ takes into account the doubling of degrees of freedom. In the following we see that this picture is partially correct also considering the subleading terms, as well as considering finite systems.
4. BEYOND THE ASYMPTOTIC BEHAVIOR

4.1 Entanglement entropy in the XX model

As we evaluated explicitly in Chapter 2, the Hamiltonian of the XX model (2.15) is diagonal in momentum space and, for $|h| < 1$, the ground-state is a partially filled Fermi sea with Fermi-momentum

$$k_F = \arccos|h|.$$  (4.8)

In the following we will always assume that $|h| < 1$ so that we are dealing with a gapless theory.

Using Wick theorem, the reduced density matrix of a block $A = [\ell_0 + 1, \ell_0 + \ell]$ composed of $\ell$ contiguous sites in the ground state of the Hamiltonian (2.15) can be written as

$$\rho_A = \det C \exp \left( \sum_{j,l \in A} \ln(C^{-1} - 1) c_j^c c_l \right),$$  (4.9)

where the correlation matrix has matrix elements $C_{nm} = \langle c_n^c c_m \rangle$. We already wrote the correlation matrix both for periodic (cf. (2.43)) and open (cf. (2.72)) boundary conditions. Choosing, for example, $J = -1$, we have

$$C_{nm} = k_F \frac{\delta_{in} + (1 - \delta_{in}) \sin(k_F(n - m))}{\pi(n - m)} - \frac{\sin(k_F(n + m))}{\pi(n + m)}.$$  (4.10)

The PBC result is recovered when $n, m \to \infty$ while keeping the distance $n - m$ finite, i.e. far from the boundary, as physical intuition suggests. In section 2.2 we found that the entanglement is related to the eigenvalues of the correlation matrix. In brief, as a real symmetric matrix, $C$ can be diagonalized by an orthogonal transformation

$$R C R^T \equiv \delta_{im}(1 + \nu_m)/2,$$  (4.11)

and the eigenvalues depend both on $\ell$ and $\ell_0$. The reduced density matrix $\rho_A$ is uncorrelated in the transformed basis, so that the Rényi entropies can be expressed in terms of the eigenvalues $\nu_l$ as

$$S_\alpha(\ell_0, \ell) = \sum_{l=1}^{\ell} c_\alpha(\nu_l), \quad \text{with} \quad c_\alpha(x) = \frac{1}{1 - \alpha} \ln \left[ \left( \frac{1 + x}{2} \right)^\alpha + \left( \frac{1 - x}{2} \right)^\alpha \right].$$  (4.12)

The above construction refers to the block entanglement of fermionic degrees of freedom. However, we have shown in section 2.2 that the Jordan-Wigner transformation, although non local, mixes only spins inside of the block. Furthermore, also in the case of XX chains with different boundary conditions (e.g. fixed) the Jordan-Wigner string would spoil the correspondence between spins and fermions for an interval detached from the boundary (i.e. $\ell_0 \neq 0$). It is a peculiarity of OBC that the reduced density matrix of any interval at any distance from the boundary is the same for spins and fermions. Indeed the equivalence relies on the parity symmetry of the boundary conditions (the Hamiltonian is already symmetric) associated to the operator $\sigma_z$ for which only the expectation value of an even number of fermions is different
4.1 Entanglement entropy in the XX model

from 0. When this not happens (e.g. when the condition reads as \( \sigma^x_L |\Psi_0\rangle = |\Psi_0\rangle \), with \( |\Psi_0\rangle \) the ground state), the products of the odd-number fermions cannot be neglected and the RDM is no longer the exponential of a simple quadratic operator, as in Eq. (2.103), because some linear terms appear in the exponential.

The sum in Eq. (4.12) can be put in the form of an integral on the complex plane \[23\], introducing the determinant

\[
D_\ell(\lambda) = \det((\lambda + 1)I - 2C) \equiv \det(G).
\]

(4.13)

In the eigenbasis of \( C \) the determinant is simply a polynomial of degree \( \ell \) in \( \lambda \) with zeros \( \{\nu_j|j = 1, \ldots, \ell\} \), i.e.

\[
D_\ell(\lambda) = \prod_{j=1}^{\ell}(\lambda - \nu_j).
\]

(4.14)

This implies that the Rényi entropies have the integral representation (cf. Eq. (2.132))

\[
S_\alpha(\ell) = \frac{1}{2\pi i} \oint d\lambda \ e^{\alpha(\lambda)} d\ln D_\ell(\lambda),
\]

(4.15)

where the contour of integration encircles the segment \([-1,1]\). In the PBC case and in the thermodynamic limit \((L \to \infty)\), Fisher-Hartwig conjecture allows to obtain the asymptotic large \( \ell \) behavior of \( S_\alpha(\ell) \) \[23\]. The generalized Fisher-Hartwig conjecture permits the computation of all harmonic corrections \[71 78\], while non-harmonic corrections can be computed exploiting random matrix techniques \[78\]. In the next subsection, we report the Fisher-Hartwig approach to PBC and the generalization to Toeplitz+Hankel matrices needed for obtaining the corrections for OBC.

4.1.1 The asymptotic result

The matrix \( G \) in Eq. (4.13) is an \( \ell \times \ell \) Toeplitz or Toeplitz+Hankel matrix depending on the boundary conditions whether periodic or open. The standard calculation of the asymptotic behavior of \( \det(G) \) proceeds as follows. We define the symbol of the structured matrix \( G_{in} = g_{l-n} - g_{l+n+s} \) to be the Fourier transform \( g(\theta) \) of \( g_l \)

\[
G_{in} = \int_0^{2\pi} \frac{d\theta}{2\pi} \left( e^{i(l-n)\theta} - e^{i(l+n+s)} \right) g(\theta),
\]

(4.16)

which in our case takes the form

\[
g(\theta) = \begin{cases} 
\lambda + 1 & \theta \in [k_F, 2\pi - k_F] \\
\lambda - 1 & \theta \in [0, k_F] \cup [2\pi - k_F, 2\pi].
\end{cases}
\]

(4.17)

On the interval \([0, 2\pi]\) the function \( g(\theta) \) has two discontinuities at \( \theta_1 = k_F \) and \( \theta_2 = 2\pi - k_F \). From the correlation matrix \[4.10\] we see that the parameter \( s \) is equal to \( 2\ell_0 + 2 \), where \( \ell_0 \) is the distance of the block from the boundary (i.e. starting from the site \( \ell_0 + 1 \)). PBC involve
4. BEYOND THE ASYMPTOTIC BEHAVIOR

the single Toeplitz part and can be obtained by sending \( s \) to infinity (indeed \( g_{\infty} \to 0 \)). The asymptotic behavior of \( \det G \) for a discontinuous symbol like the XX one is mathematically known only for \( s = 1, 2, \infty \). In the Toeplitz case (\( s \to \infty \)) it is possible to use the (generalized) Fisher-Hartwig conjecture. The other two cases \( s = 1, 2 \) have been recently studied in Ref. \[61\] where Deift, Itz, and Krasovsky generalize the Fisher-Hartwig conjecture for some kinds of Toeplitz+Hankel matrices. In fact the case \( s = 1 \) does not correspond to any physical situation \( (s = 2 \ell_0 + 2 \) must be even), however the result for \( s = 2 \) can be used to calculate the Rényi entropies of a block starting from the boundary of an open XX chain, as indeed we done in Ref. \[11\].

First of all we consider PBC, i.e. \( s \to \infty \) in Eq. (4.16). In order to employ the Fisher-Hartwig conjecture, or its generalization, one needs to express \( g(\theta) \) in the form

\[
g(\theta) = f(\theta) \prod_{r=1}^{R} e^{ib_{r}[\theta - \theta_{r} - \pi \text{sgn}(\theta - \theta_{r})]} (2 - 2 \cos(\theta - \theta_{r}))^{a_{r}}, \tag{4.18}
\]

where \( R \) is an integer, \( a_{r}, b_{r} \) and \( \theta_{r} \) are constants and \( f(\theta) \) is a smooth function with winding number zero. The Fisher-Hartwig conjecture then states that the large-\( \ell \)-asymptotic behavior of the Toeplitz determinant is

\[
D_{\ell} \sim F[f(\theta)]^{\ell} \left( \prod_{j=1}^{R} e^{a_{j}^{2} - b_{j}^{2}} \right) E, \tag{4.19}
\]

where \( F[f(\theta)] = \exp(\frac{1}{2\pi} \int_{0}^{2\pi} d\theta \ln f(\theta)) \) and \( E \) is a known function of \( f(\theta), a_{r}, b_{r}, \) and \( \theta_{r} \). In our case it is straightforward to express the symbol in the canonical form (4.18). As \( g(\theta) \) has two discontinuities in \([0, 2\pi)\) we have \( R = 2 \). By comparison, we have

\[
a_{1,2} = 0, \quad b_{2} = -b_{1} = \beta_{\lambda} + m, \quad f(\theta) = f_{0} = (\lambda + 1)e^{-2ib_{2}kF} = (\lambda + 1)e^{-2ikFr}e^{-2ikF\beta_{\lambda}}, \tag{4.20}
\]

where \( m \) is an arbitrary integer number, that labels the different inequivalent representations of the symbol \( g(\theta) \), see \[80\], and

\[
\beta = \frac{1}{2\pi i} \log \left[ \frac{\lambda + 1}{\lambda - 1} \right] = \arg \frac{\lambda + 1}{\lambda - 1} < \pi. \tag{4.21}
\]

Jin and Korepin employed the Fisher-Hartwig conjecture for the \( m = 0 \) representation and obtained the following result for the large-\( \ell \) asymptotics of \( D_{\ell}(\lambda) \) \[23\]

\[
D_{\ell}^{BC}(\lambda) \sim \left[ (\lambda + 1) \left( \frac{\lambda + 1}{\lambda - 1} \right)^{-k_{F}} \right]^{\ell} (2\ell|\sin k_{F}|)^{-2\beta_{\lambda}^{2}G^{2}(1 + \beta_{\lambda})G^{2}(1 - \beta_{\lambda})}, \tag{4.22}
\]

where \( G(x) \) is the Barnes G-function \[82\].

For the case of our piecewise symbol and for the Toeplitz+Hankel matrix corresponding to \( s = 2 \), the analogous theorem was known from longer time \[83\]. The result in Refs. \[61,83\] has
4.2 Corrections to the scaling

In this section we consider the corrections to the scaling to the asymptotic result derived in the previous section. When the symbol has several inequivalent representations, as in our case, a structure similar to the FH formula, with more constants $a_j, b_j$ corresponding to boundary terms. We specialize this formula to the symbol in Eq. (4.17), and we obtain the asymptotic behavior of the determinant $D_\ell(\lambda)$ as

$$D_\ell^{OBC}(\lambda) \sim e^{i(\frac{\pi}{2} - k_F)\beta_\lambda} \left( \lambda + 1 \right)^{-\frac{2\pi}{\lambda}} (4\ell |\sin(k_F)|)^{-\beta_\lambda} G(1 - \beta_\lambda) G(1 + \beta_\lambda), \quad (4.23)$$

Notice that the two asymptotic expressions Eq. (4.22) and Eq. (4.23) are in the following relation:

$$D_\ell^{OBC}(\lambda) \sim e^{i(\frac{\pi}{2} - k_F)\beta_\lambda} \sqrt{D_\ell^{PBC}} \quad (4.24)$$

The Rényi entropies can be obtained by inserting (4.22) or (4.23), depending on boundary conditions, into (4.15) and carrying out the integral. The factor $e^{i(\frac{\pi}{2} - k_F)\beta_\lambda}$ in Eq. (4.24) does not contribute to the entropies, indeed

$$\left(\frac{1}{2} - \frac{k_F}{\pi}\right) \frac{1}{2\pi i} \oint d\lambda \frac{c_\alpha(\lambda)}{1 - \lambda^2} = 0, \quad (4.25)$$

where we used that $c_\alpha(1) = c_\alpha(-1) = 0$ for any $\alpha$. Thus, from Eq. (4.24) and by observing that Eq. (4.15) is linear in $\log D_\ell$, we get the fundamental result

$$S_\alpha^{OBC}(\ell) \sim \frac{1}{2} S_\alpha^{PBC}(2\ell), \quad (4.26)$$

which is valid up to $O(\ell^0)$. This relation between $S_\alpha$ for periodic and open boundary conditions is exactly what expected from CFT, as reviewed in the previous section. In particular, we find that in the XX model the boundary entropy $\log g$ (see Eq. (4.1)) is zero, as it has been firstly observed in the Affleck and Ludwig’s work [75]. The asymptotic behavior of the integral (4.15) as been worked out by Jin and Korepin in Ref. [23], who found

$$S_\alpha^{PBC}(\ell) = \frac{1}{6} \left(1 + \frac{1}{\alpha}\right) \ln(2\ell |\sin k_F|) + E_\alpha, \quad (4.27)$$

where the constant $E_\alpha$ has the integral representation

$$E_\alpha = \left(1 + \frac{1}{\alpha}\right) \int_0^\infty \frac{dt}{t} \left[ \frac{1}{1 - \alpha^{-2}} \left( \frac{1}{\alpha \sinh t/\alpha} - \frac{1}{\sinh t} \right) - \frac{e^{-2t}}{6} \right]. \quad (4.28)$$

Both the leading logarithmic term and the subleading constant one are in agreement with Eq. (4.1) (with $\ln g = 0$). There is then no new physical information in this expression. However, the present result is based on a mathematical theorem and so it provides a rigorous confirmation of a general CFT result in a specific lattice model.

4.2 Corrections to the scaling

In this section we consider the corrections to the scaling to the asymptotic result derived in the previous section. When the symbol has several inequivalent representations, as in our case,
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the Fisher-Hartwig conjecture is only asymptotically correct (at least in our happy situation) and it is unable to capture the subleading behavior. In the Toeplitz case, namely for PBC, the generalized Fisher-Hartwig conjecture (gFHC) \[80\] applies, and one has to sum over all these representations as

\[ D^\text{PBC}_\ell (\lambda) \sim \sum_m (f_0(m))^{\ell} e^{-\sum_{\ell=1}^2 (b_{\ell}(m))^2 E(m)} , \tag{4.29} \]

where all the various FH constants \( f_0, b_{\ell}, \) and \( E \) depend on \( m \), as shown in Eq. \[4.20\]. Then the full result of the generalized Fisher-Hartwig conjecture for the Toeplitz determinant takes the form \[78\]

\[ D^\text{PBC}_\ell \sim (\lambda + 1)^\ell \left( \frac{\lambda + 1}{\lambda - 1} \right)^{-k_F \ell} \sum_{m \in \mathbb{Z}} (2|\sin k_F|)^{-2(m+\beta_\lambda)^2} e^{-2i k_F m \ell} \times [G(m+1+\beta_\lambda)G(1-m-\beta_\lambda)]^2 \tag{4.30} \]

The analogous generalization for the Toeplitz+Hankel matrix \[4.16\] with \( s = 2 \), namely for the XX chain with OBC, has not been proved yet, however in Ref. \[11\] we have conjectured the following formula:

\[ D^\text{OBC}_\ell (\lambda) \sim (\lambda + 1)^\ell \left( \frac{\lambda + 1}{\lambda - 1} \right)^{-k_F \ell} \sum_{m \in \mathbb{Z}} e^{\frac{i}{2} m (\beta_\lambda + m)} \left[ 4 \left( \frac{\ell}{2} \right) \sin k_F \right]^{-2(m+\beta_\lambda)^2} \times e^{-2i k_F (\beta_\lambda + m) (\ell + 1/2)} G(m+1+\beta_\lambda)G(1-m-\beta_\lambda) . \tag{4.31} \]

Most of the above formula is inspired to the gFH Eq. \[4.30\] and adapted to the present case. However, the factor \( 1/2 \) as an additive constant to \( \ell \) has been introduced without any mathematical reason. This factor \( 1/2 \) gives an analytic (i.e. non-harmonic) correction to \( D_\ell (\lambda) \) and we introduced it to reproduce accurately the numerical data. In Fig. \[4.1\] we report the ratio of the numerically calculated \( D_\ell (\lambda) \) asymptotic value with and without the additional \( 1/2 \), showing that the former converges faster. The data for the resulting entanglement entropy \( S_2 (\ell) \) (reported in the right panel of Fig. \[4.1\]) show even more clearly the importance of this factor. In any case, we conjectured this gFH formula and in doing so we prefer to conjecture an expression that reproduces numerical data as accurately as possible.

The leading corrections to the scaling is obtained by summing only the three modes \( m = -1,0,1 \), obtaining

\[ D_\ell \sim D_\ell^{(0)} (1 + \Psi_\ell (\lambda)) \tag{4.32} \]

where we isolated the leading term \[4.22\] or \[4.23\], depending on boundary conditions, and

\[ \Psi_\ell (\lambda) = \begin{cases} e^{-2ik_F L_k^{-2-4\beta}} \frac{\Gamma((1+\beta)}{\Gamma(1-\beta)} - e^{2ik_F e^{2ik_F \ell} L_k^{-2+4\beta}} \frac{\Gamma(1+\beta)}{\Gamma(1-\beta)} & \text{PBC} \\ ie^{-ik_F e^{-2ik_F \ell} L_k^{-1-2\beta}} \frac{\Gamma((1+\beta)}{\Gamma(1-\beta)} - ie^{ik_F e^{2ik_F \ell} L_k^{-1+2\beta}} \frac{\Gamma(1+\beta)}{\Gamma(1-\beta)} & \text{OBC}. \end{cases} \tag{4.33} \]

\( L_k \) is defined as

\[ L_k = \begin{cases} 2\ell |\sin(k_F)| & \text{PBC} \\ 2(2\ell + 1)|\sin(k_F)| & \text{OBC}. \end{cases} \tag{4.34} \]
4.2 Corrections to the scaling

Figure 4.1: Asymptotic of determinants - Left: The ratio \( R = D_\ell(\lambda)/D_\ell^{(0)}(\lambda) \) for \( \lambda = 1 + i \) and \( k_F = \sqrt{\pi}/2 \). Right: The entanglement entropy for \( k_F = \sqrt{\pi}/2 \). Both graphs show the importance of the additive factor 1/2.

We define

\[
d_\alpha(\ell) \equiv S_\alpha(\ell) - S_\alpha^{(0)}(\ell),
\]

with \( S_\alpha^{(0)} \) the leading behavior of the Rényi entropies, i.e. Eq. (4.27) for PBC and a slightly modified expression for OBC (cf. Eq. (4.26)), which takes into account the shift of \( \frac{1}{2} \) in the subsystem’s length:

\[
S_\alpha^{(0)}_{\mathrm{OBC}} = \frac{1}{12} \left( 1 + \frac{1}{\alpha} \right) \ln \left[ 2 (2\ell + 1) \sin |k_F| \right] + \frac{E_\alpha}{2}.
\]

For large \( L_k \) we have

\[
d_\alpha(\ell) \sim \frac{1}{2\pi i} \oint d\lambda \frac{\ln [1 + \Psi_\ell(\lambda)]}{d\lambda} = \frac{1}{2\pi i} \oint d\lambda \frac{d\Psi_\ell(\lambda)}{d\lambda} + \ldots.
\]

The contour integral can be written as the sum of two contributions infinitesimally above and below the interval \([-1, 1]\) respectively, i.e.

\[
d_\alpha(\ell) \sim \frac{1}{2\pi i} \left[ \int_{1+i\epsilon}^{1-i\epsilon} - \int_{1-i\epsilon}^{1+i\epsilon} \right] d\lambda \frac{d\Psi_\ell(\lambda)}{d\lambda}.
\]

This shows that we only require the discontinuity across the branch cut. The only discontinuous function is \( \beta_\lambda \), which for \(-1 < x < 1\) behaves as

\[
\beta_{x \pm \epsilon} = -i w(x) \mp \frac{1}{2}, \quad \text{with} \quad w(x) = \frac{1}{2\pi} \ln \frac{1 + x}{1 - x}.
\]

We now change variables from \( \lambda \) to \( w \)

\[
\lambda = \tanh(\pi w), \quad -\infty < w < \infty.
\]
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For PBC we have
\[
\begin{align*}
\left[ L_k^{-2-4\beta} \frac{\Gamma^2(1+\beta)}{\Gamma^2(-\beta)} \right]_{\beta=-iw-\frac{1}{2}} & \sim L_k^{4\alpha w} \gamma^2(w), \\
\left[ L_k^{-2+4\beta} \frac{\Gamma^2(1-\beta)}{\Gamma^2(-\beta)} \right]_{\beta=-iw+\frac{1}{2}} & \sim -L_k^{-4\alpha w} \gamma^2(-w),
\end{align*}
\]
while for OBC we get
\[
\begin{align*}
\left[ L_k^{-1-2\beta} \frac{\Gamma(1+\beta)}{\Gamma(-\beta)} \right]_{\beta=-iw-\frac{1}{2}} & \sim L_k^{2\alpha w} \gamma(w), \\
\left[ L_k^{-1+2\beta} \frac{\Gamma(1-\beta)}{\Gamma(-\beta)} \right]_{\beta=-iw+\frac{1}{2}} & \sim -L_k^{-2\alpha w} \gamma(-w),
\end{align*}
\]
where we have dropped terms of order $O(L_k^{-2})$ compared to the leading ones and we have defined
\[
\gamma(w) = \frac{\Gamma(\frac{1}{2} - iw)}{\Gamma(\frac{1}{2} + iw)}. \tag{4.43}
\]

Integrating by parts and using
\[
\frac{d}{dw} \Gamma(\pi w) = \frac{\pi\alpha}{1-\alpha} \left( \tanh(\alpha\pi w) - \tanh(\pi w) \right), \tag{4.44}
\]
we arrive at
\[
d_{\alpha}(\ell) \sim \frac{i\alpha}{2(1-\alpha)} \int_{-\infty}^{\infty} dw (\tanh(\pi w) - \tanh(\alpha\pi w)) W_1(w) \tag{4.45}
\]
where
\[
W_1(w) = \begin{cases} 
-2i\kappa P L_k^{4\alpha w} \gamma^2(w) - e^{2ik\ell}\ell^{-4\alpha w} \gamma^2(-w) & \text{PBC} \\
\frac{ie^{-ik\ell}}{e^{2ik\ell}} L_k^{2\alpha w} \gamma(w) + ie^{-ik\ell} e^{2ik\ell} L_k^{-2\alpha w} \gamma(-w) & \text{OBC}.
\end{cases} \tag{4.46}
\]

For large $\ell$ the leading contribution to the integral arises from the poles closest to the real axis. These are located at $w_0 = i/2\alpha$ ($w_0 = -i/2\alpha$) for the first (second) term in both cases. Evaluating their contributions to the integral gives
\[
d_{\alpha}(\ell) \sim \begin{cases} 
\frac{2\cos[2k\ell]}{1-\alpha} 2\ell \sin k\ell |^{-2/\alpha} \Gamma(\frac{1}{2} + \frac{\alpha}{2}) + o(\ell^{-2/\alpha}) & \text{PBC} \\
\frac{2\sin[2k\ell(2\ell+1)]}{1-\alpha} 2(2\ell+1) \sin k\ell |^{-1/\alpha} \Gamma(\frac{1}{2} + \frac{\alpha}{2}) + o(\ell^{-1/\alpha}) & \text{OBC}.
\end{cases} \tag{4.47}
\]

In Fig. 4.2 we report the numerical calculated $S_{\alpha}(\ell)$ for a semi-infinite chain and for small values of $\alpha = 1, 2, 3$. For these values of $\alpha$, the inclusion of only the first correction to the scaling (as in Eq. (4.44)) is enough to describe very accurately $S_{\alpha}(\ell)$ even for relatively small values of $\ell$. The figure shows the correctness also of the $k\ell$ dependence of the correction, that is the most important difference compared to PBC. Notice that without the factor $1/2$ introduced by hand in Eq. (4.31), the correction (4.47) would be inadequate at order $1/\ell$, as anticipated in Fig. 4.4.
4.2 Corrections to the scaling

Figure 4.2: Leading correction - \( S_\alpha(\ell) \) in a semi-infinite XX chain for \( \alpha = 1, 2, 3 \) and two different values of \( k_F \) specified in the captions. The exact numerical results are compared with the asymptotic formula including only the first correction to the scaling. For these small values of \( \alpha \), the agreement is excellent. Notice the incommensurability effects when \( k_F \) is not a fraction of \( \pi \) (right graph).

4.2.1 Subleading corrections

Eq. (4.47) describes the asymptotic behavior in the limit \( L_k \to \infty \) with \( \alpha \) fixed. It provides a good approximation for large finite \( \ell \) as long as \( \ln(L_k) \gg \alpha \). For practical purposes it is useful to know the corrections to \( S_\alpha(\ell) \) for large \( \ell \) but \( \ln(L_k) \) not necessarily much larger than \( \alpha \). In this regime there are two main sources of corrections to (4.47). The integral (4.44) is no longer dominated by the poles closest to the real axis and contributions from further poles need to be included. These give rise to corrections proportional to \( L_k^{-2q/\alpha} \) (PBC) or \( L_k^{-q/\alpha} \) (OBC), with \( q \) integer. Furthermore, terms in the expansion of the logarithm in Eq. (4.37) need to be taken into account. The corresponding contributions are proportional to \( e^{\pm i2p k_F \ell} \) with \( p = 2, 3, \ldots \).

We now take both types of corrections into account. We first consider the series expansion of the logarithm in Eq. (4.37).

\[
\ln \left[ 1 + \Psi_\ell(\lambda) \right] = \sum_{p=1}^{\infty} \frac{(-1)^{p+1} (\Psi_\ell(\lambda))^p}{p}.
\] (4.48)

Recalling the explicit expression (4.33) for \( \Psi_\ell(\lambda) \) leads to a binomial sum

\[
(\Psi_\ell(\lambda))^p = \begin{cases}
\sum_{q=0}^{p} \binom{p}{q} e^{2ik_F \ell(2q-p)} L_k^{-2p} L_k^{-4(p-2q)\beta_\lambda} c_{p,\beta} c_{q,\beta}^\text{PBC} \\
\sum_{q=0}^{p} \binom{p}{q} (-1)^q e^{ik_F \ell(2q-p)} L_k^{-2p} L_k^{-(p-2q)\beta_\lambda} c_{p,\beta} c_{q,\beta}^\text{OBC},
\end{cases}
\] (4.49)

where we have introduced the shorthand notation \( c_\beta = \Gamma(1 + \beta)/\Gamma(-\beta) \).

When calculating the discontinuity across the branch cut running from \( \lambda = -1 \) to \( \lambda = 1 \) all terms other than \( q = 0 \) and \( q = p \) give rise to terms that are subleading in \( L_k \). Hence we may approximate

\[
(\Psi_\ell(\tanh(\pi w) + i\epsilon))^p - (\Psi_\ell(\tanh(\pi w) - i\epsilon))^p \approx W_p(w)
\] (4.50)
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with

\[ W_p(w) = \begin{cases} 
  e^{-2ik_Fp}L_k^{4iw\gamma_{2p}}(w) - e^{2ik_Fp}L_k^{-4iw\gamma_{2p}}(-w) & \text{PBC} \\
  ipe^{-2ik_Fp(\ell + 1/2)p}L_k^{2iw\gamma_{p}}(w) - (-i)e^{2ik_Fp(\ell + 1/2)p}L_k^{-2iw\gamma_{p}}(-w) & \text{OBC}
\end{cases} \quad (4.51) \]

Plugging this into Eq. (4.37) we get

\[ d_\alpha(\ell) \sim \sum_{p=1}^{\infty} \frac{(-1)^{p+1}}{p} \frac{in}{2(1-\alpha)} \int_{-\infty}^{\infty} dw (\tanh(\pi w) - \tanh(\alpha \pi w)) W_p(w) . \quad (4.52) \]

The integral is carried out by contour integration, taking the two terms in \( W_p(w) \) Eq. (4.51) into account separately. The first (second) contribution has simple poles in the upper (lower) half plane at \( w_q = i \frac{2q-1}{2\alpha} \) (\( w_q = -i \frac{2q-1}{2\alpha} \)), where \( q \) is a positive integer such that \( 2q-1 \neq \alpha, 3\alpha, 5\alpha, \ldots \) for \( \alpha \neq 1 \). Contour integration then gives

\[ d_\alpha(\ell) = \frac{1}{1-\alpha} \sum_{q=1}^{\alpha-1} \left\{ \log \left( 1 + 2\cos(2k_F\ell)L_k^{-2q-1}Q_{\alpha,q} + L_k^{-4q-1}Q_{\alpha,q}^4 \right) \right\} PBC \]

\[ d_\alpha(\ell) = \frac{1}{1-\alpha} \sum_{q=1}^{\alpha-1} \left\{ \log \left( 1 + 2\sin(2k_F(\ell + \frac{1}{2}))L_k^{-2q-1}Q_{\alpha,q} + L_k^{-4q-1}Q_{\alpha,q}^4 \right) \right\} OBC , \quad (4.53) \]

where we defined the constants \( Q_{\alpha,q} \) as

\[ Q_{\alpha,q} = \frac{\Gamma(\frac{1}{2} + \frac{2q-1}{2\alpha})}{\Gamma(\frac{1}{2} - \frac{2q-1}{2\alpha})} . \quad (4.54) \]

Eq. (4.53) is correct up to \( O(\ell^{-1}) \). It shows that there are contributions to the Rényi entropies with oscillation frequencies that are arbitrary multiples of \( 2k_F \). In all the above analysis we have ignored contributions to the generalized Fisher-Hartwig conjecture with \( |m| > 1 \). While these lead to oscillatory contributions with frequencies that are integer multiples of \( 2k_F \) they are suppressed by additional powers of \( \ell^{-1} \) and hence are subleading, even in the case where \( \alpha \) is not small.

In Fig. 4.3 we show the corrections \( d_\alpha(\ell) \) for \( \alpha = 20 \) and 50 in the open chain with \( k_F = \pi/6 \) and \( \pi/2 \) respectively and their comparison with the asymptotic result Eq. (4.53). Step by step we take into account further terms in the asymptotic expression until we obtain a satisfying agreement with the numerical data. For \( \alpha = 20, 13 \) terms in Eq. (4.53) are enough to reproduce the data, while for \( \alpha = 50 \) we need 41 terms to have the same accuracy. These numbers are larger than the corresponding ones for PBC [78] because the corrections in the present case have smaller exponents.

4.2.2 The limit of large \( \alpha \)

\( S_\infty(\ell) \) is known in the literature as single copy entanglement [53][85]. In fact, the limit \( \alpha \to \infty \) also provides information on the behavior of \( S_\alpha(\ell) \) in the regime \( \alpha \gg \ln L_k, L_k \gg 1 \). Notice that it is necessary to sum up an infinite number of contributions in order to extract the large-\( \ell \) asymptotics. In Refs. [78] and [11] the asymptotic result has been derived by taking the parameter \( \alpha \) to infinity and then carrying out the resulting integrals in Eq. (4.52). Here we
4.2 Corrections to the scaling

Figure 4.3: Subleading corrections - Difference between the Rényi entanglement entropy and its asymptotic value for \( n = 20 \) (left) and 50 (right) with \( k_F = \pi/6 \) and \( \pi/2 \). The exact numerical data are compared with the series expansion of Eq. (4.53) with increasing number of terms. For \( n = 50 \) we report curves with 1, 3, 5, 9, 15, 25, 41 terms, while for \( n = 20 \) we consider 1, 2, 3, 5, 8, 13 terms. Increasing the number of terms considered, the expansion (4.53) becomes accurate even for values of \( \ell \) as small as 2.

follow a different approach. Indeed, the limit can be obtained directly from Eq. (4.53), turning the sum into an integral by means of the Euler-Maclaurin formula:

\[
\lim_{\ell \to \infty} \frac{d}{d\ell} \left( \frac{e^{2\gamma L_k}}{2\log L_k} \right) = \int_0^{s_k} \frac{dx}{s_k} \left\{ \log \left[ 1 + 2 \cos(2k_F\ell) e^{-2x} \gamma \left( \frac{ix}{s_k^2} \right) + e^{-4x} \gamma^2 \left( \frac{ix}{s_k^2} \right) \right] \right\} \quad \text{PBC}
\]

\[
\lim_{\ell \to \infty} \frac{d}{d\ell} \left( \frac{e^{2\gamma L_k}}{2\log L_k} \right) = \int_0^{s_k} \frac{dx}{s_k} \left\{ \log \left[ 1 + 2 \sin(2k_F\ell + \frac{1}{2}) e^{-2x} \gamma \left( \frac{ix}{s_k^2} \right) + e^{-4x} \gamma^2 \left( \frac{ix}{s_k^2} \right) \right] \right\} \quad \text{OBC},
\]

where \( s_k = \log L_k \). The upper limit of integration can be sent to \( \infty \), up to corrections \( O(L_k^{-1}) \).

Then, \( \gamma \left( \frac{ix}{s_k^2} \right) \) can be series expanded in powers of \( s_k \) in order to get the correction up to the desired order \( O((\log L_k)^{-1}) \). The leading order can be obtained by substituting the function \( \gamma \) with 1:

\[
\lim_{\ell \to \infty} \frac{d}{d\ell} \left( \frac{e^{2\gamma L_k}}{2\log L_k} \right) = \int_0^{s_k} \frac{dx}{s_k} \left\{ \log \left[ 1 + 2 \cos(2k_F\ell) e^{-2x} \left( \frac{ix}{s_k^2} \right) + e^{-4x} \left( \frac{ix}{s_k^2} \right)^2 \right] \right\} \quad \text{PBC}
\]

\[
\lim_{\ell \to \infty} \frac{d}{d\ell} \left( \frac{e^{2\gamma L_k}}{2\log L_k} \right) = \int_0^{s_k} \frac{dx}{s_k} \left\{ \log \left[ 1 + 2 \sin(2k_F\ell + \frac{1}{2}) e^{-2x} \left( \frac{ix}{s_k^2} \right) + e^{-4x} \left( \frac{ix}{s_k^2} \right)^2 \right] \right\} \quad \text{OBC},
\]

where \( \text{Li} \) is the polylogarithm.

Summing some of the subleading terms in (4.55) to all orders in \( (\log L_k)^{-1} \) leads to an expression of the form

\[
\frac{d}{d\ell} \left( \frac{e^{2\gamma L_k}}{2\log L_k} \right) \sim \frac{1}{\log(4e^\gamma L_k)} \left\{ \text{Li}_2(-e^{-4k_F\ell}) + \text{Li}_2(-e^{-2k_F\ell}) + \text{Li}_2\left( \frac{e^{2k_F\ell}}{2} \right) + \text{Li}_2\left( \frac{e^{4k_F\ell}}{2} \right) \right\} \quad \text{PBC}
\]

\[
\frac{d}{d\ell} \left( \frac{e^{2\gamma L_k}}{2\log L_k} \right) \sim \frac{1}{\log(4e^\gamma L_k)} \left\{ \text{Li}_2(-e^{-4k_F\ell}) + \text{Li}_2(-e^{-2k_F\ell}) + \text{Li}_2\left( \frac{e^{2k_F\ell}}{2} \right) + \text{Li}_2\left( \frac{e^{4k_F\ell}}{2} \right) \right\} \quad \text{OBC},
\]

where \( \gamma \) is the Euler’s constant, so that \( 4e^\gamma \approx 7.12429 \). Notice that if \( k_F \) is in a rational ratio with \( \pi \), the expressions written in terms of the polylogarithms in Eq. (4.55) identify a finite number of curves: e.g. for \( k_F = \frac{\pi}{2} \) the correction distinguishes between even and odd lengths.

To check this result, in Fig. 4.4 we report the exact numerical data (only for \( k_F = \pi/2 \) and OBC) for \( 1/|d_\infty(\ell)| \) in log-linear scale, showing explicitly the logarithmic form of the corrections, described very precisely by Eq. (4.57).
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Figure 4.4: Single copy entanglement - $1/|d_{\infty}(\ell)|$ with $d_{\infty}(\ell) = S_{\infty}(\ell) - S_{\infty}^{(0)}(\ell)$ vs $\ell$ in log-linear scale for $k_F = \pi/2$. Corrections to the scaling are logarithmic and perfectly described by Eq. (4.57), represented as two straight lines for $\ell$ even and odd respectively.

4.3 Finite systems

From the correlation matrices (2.43) (PBC) and (2.72) (OBC), it is straightforward to obtain numerical results for $S_\alpha(\ell)$ also in finite systems. This analysis has been done with considerable numerical accuracy in Refs. [76,86] for the Von Neumann entanglement entropy and in Ref. [76] for general $\alpha$. However, the accurate results for the amplitudes of the corrections to the scaling were not compared with theoretical predictions, not available at that time.

The modification of the leading term in Eq. (4.3) (PBC) and Eq. (4.4) (OBC) for finite systems is provided by conformal field theory [5]: the Rényi entropies are given by Eqs. (4.3) and (4.4), where the length of the subsystem $\ell$ is substituted by the chord distance $L/\pi \sin(\pi \ell/L)$.

However, we would like an expression that takes into account corrections to the scaling and that is accurate at order $1/\ell$, while we keep fixed the ratio $\ell/L$. This is beyond the predictive power of CFT, but an intuitive argument to find a proper modification of Eq. (4.4) valid in finite size can be given, leading to the expressions:

$$S^{\text{PBC}}_\alpha(\ell) = \frac{1}{6} \left( 1 + \frac{1}{\alpha} \right) \ln \left[ \frac{L}{\pi} \sin \frac{\pi L}{L} |\sin k_F| \right] + E_\alpha$$

$$+ \frac{2 \cos[2k_F \ell]}{1 - \alpha} \left\{ \left[ \frac{2 L}{\pi} \sin \frac{\pi L}{L} |\sin k_F| \right]^{-1/\alpha} \frac{\Gamma \left( \frac{1}{2} + \frac{1}{2\alpha} \right)}{\Gamma \left( \frac{1}{2} - \frac{1}{2\alpha} \right)} \right\}^2$$  (4.58)
4.3 Finite systems

Figure 4.5: Mapping into a periodic chain - Embedding of the open finite chain in a periodic one. The blue points correspond to the original chain, the red ones are the mirror symmetric sites, while the two yellow points at $x = 0$ and $x = L + 1 \equiv -L - 1$ are “auxiliary sites”. The picture shows a block with $\ell = 2$ in the open chain corresponding to $2\ell + 1 = 5$ in the periodic one.

\[ S_\alpha^{OBC}(\ell) = \frac{1}{12} \left( 1 + \frac{1}{\alpha} \right) \ln \left[ \frac{4(L+1)}{\pi} \sin \frac{\pi(2\ell + 1)}{2(L+1)} |\sin k_F'| \right] + \frac{E_\alpha}{2} \]

\[ + \frac{2 \sin |k_F'(2\ell + 1)|}{1 - \alpha} \left[ \frac{4(L+1)}{\pi} \sin \frac{\pi(2\ell + 1)}{2(L+1)} |\sin k_F'| \right]^{-1/\alpha} \frac{\Gamma\left(\frac{1}{2} + \frac{1}{2\alpha}\right)}{\Gamma\left(\frac{1}{2} - \frac{1}{2\alpha}\right)}. \]  

(4.59)

Eq. (4.58) for periodic chains is the direct result of the substitution of $\ell$ with the chord distance in any scaling factor: the oscillatory terms with wave length comparable with the lattice spacing are not scaling. On the other hand, the expression (4.59) for open chains need a little more caution. The argument proceeds as follows. While we take the continuum limit from the spin-chain to the CFT, there is a well-known arbitrariness on the exact correspondence between the lattice sites and the coordinate on the continuum space. While for PBC, translational invariance guarantees that we can start the lattice in an arbitrary point, this is no longer true in the presence of boundaries. For a semi-infinite system, the exact result (4.4) suggests that the first site of the chain should be placed at position $x = 1$ in the continuum theory. Indeed, when building the mirror image (as usually done in boundary CFT), we have a mirror chain starting from $-1$ going up to $-\infty$. This implies that an “auxiliary site” should be introduced at $x = 0$. In this way, we have an infinite chain with a block of length $2\ell + 1$, exactly as Eq. (4.4) suggests. When we move to a finite chain of length $L$, the mirror construction is graphically depicted in Fig. 4.5. We clearly have to add another auxiliary site at the other boundary to embed the open chain in a periodic one. The resulting length of the periodic chain is $2(L + 1)$. Thus this argument suggests that from the semi-infinite formula (4.4), we can obtain a finite-size ansatz by replacing $2\ell + 1$ with the modified chord length $\frac{2(L+1)}{\pi} \sin \frac{\pi(2\ell + 1)}{2(L+1)}$. In doing so,
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Figure 4.6: Finite open systems - $S_\alpha(\ell)$ in a finite XX chain of length $L$ for $\alpha = 1, 2, 3$ and two different values of $k_F$. The exact numerical results for any $\ell$ are compared with the asymptotic formula including the first correction to the scaling. The excellent agreement confirms the effectiveness of the finite-size scaling ansatz Eq. (4.59).

we should also keep in mind that the prefactor of the correction $\sin[k_F(2\ell + 1)]$ is not scaling (as for PBC) and $\ell$ should be left unchanged. All these ingredients lead to Eq. (4.59).

In Fig. 4.6, we report numerical calculated $S_\alpha(\ell)$ for finite open systems of different lengths and for different values of $k_F$. In all cases, for $\alpha = 1, 2, 3$, when the first correction describes accurately the numerics for semi-infinite systems, we found perfect agreement between analytical and numerical results, confirming the validity of the non-rigorous argument reported above. Notice that when $k_F$ is not a simple number, as in the two graphics in the bottom of Fig. 4.6, the numerical data (points) show apparently strange periodicity. When the asymptotic exact forms are plotted (continuous lines), it is clear that the periodicity is the correct one and the previous effect is only due to the the value of $k_F$.

Notice that at $\alpha = 1$, the unusual correction in $\ell^{-1/\alpha}$ and the analytic one coming from expanding $2\ell + 1$ in the leading term are of the same order $1/\ell$.

4.4 Block disconnected from the boundary

We consider in this section the Rényi entanglement entropies for a block disconnected from the boundary in the semi-infinite chain. The numerical calculations are straightforward and can be done exactly in the same way as before just by considering the correlation matrix $C_{mn}$ starting from a spin different from the first. We stress once again that the calculation of the spin entanglement can be done simply in terms of fermions, as a peculiarity of the chain with open boundary conditions. In the case of two intervals in a PBC chain, we have seen in the previous chapters that the entanglement of spins and fermions are different [29] and also other boundary conditions are generally expected to make spins and fermions inequivalent, so that the calculations should be done following the general method, introduced in Ref. [9], to tackle with the Jordan-Wigner string.
4.4 Block disconnected from the boundary

Figure 4.7: $F_2(x)$ in the open chain - The function $F_2^{\text{lat}}(x)$ in a semi-infinite chain for different lengths of the block $\ell$. Finite $\ell$ corrections are large.

For simplicity we will consider only systems in the thermodynamic limit (i.e. semi-infinite) and at half filling ($k_F = \pi/2$), but the results are very general. In Fig. 4.7, we report the function $F_2^{\text{lat}}(x)$ obtained dividing $\text{Tr} \rho_2^2 A$ by the scaling factor in Eq. (3.2), i.e.

$$F_2^{\text{lat}}(x) \equiv \frac{\text{Tr} \rho_2^2}{c^2 (\frac{1}{\ell^2} + \frac{1}{\ell_0^2} + \frac{1}{\ell_0^2} \ell_0)^{c/8}}$$ (4.60)

where $x$ is the 4-point ratio in Eq. (3.3). Global conformal invariance implies that $F_2(x)$ is a function only of $x$, while in the figure we clearly see different curves for different $\ell$. These differences are due to finite $\ell$ and $\ell_0$ effects that are severe. In Ref. [70], it has been shown that finite $\ell$ corrections are generically of the same form (i.e. governed by the same unusual exponent) independently of the number of blocks (that in the present case generalizes to its location). Notice that the data in Fig. 4.7 are not asymptotic also because the various curves do not have the conformal symmetry $x \rightarrow 1 - x$, as discussed in Chapter 3.

We can now proceed to the calculation of the asymptotic value of the function $F_\alpha(x)$ for various $\alpha$, by using that corrections to the scaling are of the form $\ell^{-1/\alpha}$. In Fig. 4.8, we report for $\alpha = 1, 2, 3, 5$ the function $F_\alpha^{\text{lat}}(x)$ at fixed $x$, obtained numerically as explained above, as function of $\ell^{-1/\alpha}$. For large enough $\ell$, the points are aligned on straight lines, confirming the correctness of the finite $\ell$ scaling (increasing $n$, more corrections of the form $\ell^{-q/\alpha}$ must be included to reproduce the numerical data, as obvious). This allows to extrapolate to $\ell \rightarrow \infty$. The result is evident from Fig. 4.8:

$$F_\alpha(x) = 1,$$ (4.61)

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Figure 4.8: Scaling of $F_\alpha(x)$ - Scaling of the finite $\ell$ corrections for $S_\alpha(\ell)$ vs $\ell^{-1/\alpha}$ for $\alpha = 1, 2, 3, 5$. Leading corrections are of the expected form $\propto \ell^{-1/\alpha}$ and the extrapolation to $\ell \to \infty$ clearly gives $F_\alpha(x) = 1$ identically. For large values of $n$, subleading corrections $\propto \ell^{-q/\alpha}$ must be included.
identically. At first, this can seem very strange when compared with the complicated functions found for two intervals in the XX model with PBC (cf. Eq. (3.57) [9,14,28]). The simplicity of this result is due to the fact that (in the present case) spins and fermions are equivalent. For PBC free-fermions, the explicit computation shows \( F_\alpha(x) = 1 \) [72] (as confirmed in some numerical works [69]). The main peculiarity of OBC is not \( F_\alpha(x) = 1 \), but the equivalence of fermions and spins.

In this chapter we provided a number of exact results for the asymptotic scaling of the R"enyi entanglement entropies in XX spin-chains. We derive rigorously, on the basis of some mathematical theorems for the determinant of Toeplitz and Toeplitz plus Hankel matrices, the asymptotic behavior of the entanglement entropies of a block starting from the boundary of a semi-infinite system, and in an infinite system. In the case of OBC, we conjectured a generalized Fisher-Hartwig form for these determinants. We obtained the exact asymptotic behavior of \( S_\alpha(\ell) \) at order \( o(\ell^{-1}) \) for any \( n \). By combining these results with conformal field theory arguments, we derived exact expressions also in finite chains in Eqs. (4.58) and (4.59). In the case of a block detached from the boundary, we derived an exact expression for the asymptotic \( S_\alpha \) given by Eq. (3.2) with \( F_\alpha(x) = 1 \). This chapter concludes the analysis of the entanglement entropies in the ground state of spin chains. In critical systems the entanglement entropies grow as the logarithm of the characteristic length \( \ell \), otherwise they are independent of \( \ell \). In the next chapter we query whether these are peculiar features of the ground state of spin chains (with short-range interaction) or some excited states display the same properties.
4. BEYOND THE ASYMPTOTIC BEHAVIOR
5. Entanglement entropy of excited states

In Chapter 1 we have shown that the entanglement entropy of a subsystem in the ground state of a local Hamiltonian satisfies generally the area law or, in critical systems, diverges as the logarithm of the subsystem’s length (see Eq. (1.34)). In particular it does not have an extensive part. For these reasons the entanglement entropy is one of the best indicators of critical properties of extended quantum systems.

In this chapter we consider the entanglement entropy of excited states. Naive arguments suggest that the entanglement in an excited state should behave as in the ground state, as long as its energy is sufficiently low. However, in general, one expects extensive behavior: given a local Hamiltonian $H$, we can construct an infinite number of non-local Hamiltonians commuting with $H$, for example any function $f(H)$. Because the interaction is non-local, the correlation functions in the ground state of such Hamiltonians do not fall off with the distance, hence also the degrees of freedom in the internal part of the subsystem contribute to the entanglement, resulting in extensive entanglement entropy. However non-extensive states appear also at high energy. This distinction becomes less clear considering finite systems. While the states in which the entropy grows as the logarithm of $\ell$ (as long as $\ell \ll L$) are expected to behave as ground states of conformal systems, in which the length $\ell$ is replaced by the chord distance $\frac{L}{2} \sin \frac{\pi \ell}{L}$ (as we are going to show), the behavior of the entropy in the “extensive states” is difficult to predict.

Here we show some of the results obtained in Ref. [10], considering the XY spin chain in a transverse magnetic field. We employ the well-known mapping of the model to free fermions to reduce the calculation of the entanglement entropy to that of the eigenvalues of a Toeplitz matrix on the lines of the ground-state case (see Sec. 2.2). In the present computation, the properties of the excitations above the ground state will strongly affect the form of the reduced density matrix and of the entanglement entropy.

In the study of the entanglement properties of excited states, a first subtle point is the choice of the basis of the Hilbert space. In fact, while the ground state of a local Hamiltonian is usually unique (or with a finite small degeneracy, when some symmetry is not spontaneously broken), the excited states can be highly degenerate. Thus, any linear combination of them
5. ENTANGLEMENT ENTROPY OF EXCITED STATES

is still an eigenstate. In principle the entanglement properties can vary a lot with the basis. However, some features are general, e.g. the appearance of states with extensive and logarithmic entropy. We choose a basis independent of the dispersion relation. This is not only an academic subtlety, because the exact studies one can perform are limited to integrable models, for which it is well-known that the degeneracy is large. Oppositely, any small integrability breaking term will remove these degenerations and one could wonder whether the specific properties found are only features of integrable models.

The quantification of the entanglement in excited states can have consequences in the understanding of the quantum out-of-equilibrium physics and in particular of the dynamical problems known as quantum quenches, which we’ll discuss in Chapter 7. After a global quench, the entanglement entropy first increases linearly with the time and then saturates to a value proportional to the length of the block \( \ell \) \([15]\). The excited states having an extensive entanglement entropy could be the relevant ones for quench problems. Oppositely in local quantum quenches the asymptotic state displays a logarithmic entanglement entropy \([87]\) and a different class of states should be relevant.

5.1 Excited states in the XY model

The exact diagonalization of the XY model \((2.9)\) gives not only the ground-state properties but a complete classification of all the eigenstates with their energy. In the basis of free fermions, the excited states are classified according to the occupation numbers of the single-particle basis (that is the basis of Slater determinants). A generic eigenstate can be written as

\[
|E_x\rangle \equiv \prod_{k \in E_x} b_k^\dagger |0\rangle, \quad \text{with energy } E_{E_x} = \frac{1}{2} \left( \sum_{k \in E_x} \varepsilon_k - \sum_{k \notin E_x} \varepsilon_k \right),
\]

(5.1)

where \(E_x\) is the set of occupied momenta. To give a simple pictorial representation of these states, we indicate with up-arrows the occupied single-particle levels (excited quasiparticles) and with down-arrows the empty ones, with the first arrow corresponding to momentum \(\varphi_k = -\pi\).

When a set of \(n\) consecutive momenta are occupied (empty), we simply replace the up (down) string with \(\uparrow^n\) (\(\downarrow^n\)). For example, the ground state is \(|\downarrow \ldots \downarrow\rangle = |\downarrow^N\rangle\). Counting all the possible arrow orientations, it is obvious that this graphical representation generates all the \(2^N\) eigenstates of the chain. Notice that these arrows have nothing to do with the state of the spin in real space (the real space configuration is an highly entangled superposition).

When calculating the entanglement entropy, three different length scales enter in the computation: the size of the chain \(N\), the length of the block \(\ell\) and the number of excited quasiparticles that is encoded in the size \(|E_x|\) of the set \(E_x\). General results can be obtained in the thermodynamic limit \(L \to \infty\) and when \(\ell \gg 1\) (in finite size, this limit describes the regime \(L \gg \ell \gg 1\)). It is obvious that if only a small number of quasiparticle levels are populated (i.e. \(|E_x| \ll L\)), the corrections to the ground-state correlation matrix can be generally treated perturbatively.
5.1 Excited states in the XY model

and in a first approximation the excited quasiparticles contribute independently to the entanglement, giving rise to a negligible contribution in $1/L$. In Ref. [88] Alcaraz, Ibanez, and Sierra analyzed the Rényi entropies $S_\alpha$ of low-energy excitations associated to primary fields obtaining that the excess of entanglement is a finite-size scaling function related to the $2\alpha$-point correlator of the primary field. In particular, in the limit $\ell \ll L$, they have found the behavior

$$
\text{Tr}\rho_{\text{exc}}^\alpha/\text{Tr}\rho_{\text{GS}}^\alpha \sim 1 + \frac{h + \bar{h}}{3} \left( \frac{1}{\alpha} - \alpha \right) \frac{\pi^2 \ell^2}{L^2} + O\left((\ell/L)^{2\Delta}\right),
$$

(5.2)

where $\Psi$ is the operator with the smallest scaling dimension $\Delta$, and $h$ is the scaling dimension of the primary field associated to the excitation. Thus, in the thermodynamic limit, all entanglement properties of these states are equivalent to those of the ground-state, however there are interesting finite-size behaviors. Here instead we are interested in those states that are macroscopically different from the ground-state and that will have an entanglement entropy that in the thermodynamic limit could differ strongly from Eq. (1.34).

In order to work directly in the thermodynamic limit, we need a proper description of excited states. This is rather straightforward. In fact, when $L \to \infty$ the possible values of $k$ are all the integer numbers, and the reduced momentum $\varphi_k$ becomes a continuous variable $\varphi$ living in the interval $\varphi \in [-\pi, \pi]$. We are here interested in the case with $|E_x| \sim L$ (that can be seen as an “highly excited state”, even if it is not the energy that matters). Thus in all the formulae involving sums over populated energy levels, we substitute sums with integrals by using as distribution a proper defined regularized characteristic function $m(\varphi)$ that we will indicate as $m(\varphi)$. The function $(1 + m(\varphi))/2$ represents the average occupation of levels in an infinitesimal shell around the momentum $\varphi_k = 2\pi k/L$. Let us give several examples to make this limiting procedure clear ($\alpha < 1$):

$$
|\downarrow^N\rangle \longrightarrow m(\varphi) = -1,
$$

$$
|\downarrow^{N/2}\uparrow^{N/2}\rangle |\downarrow^{(1-\alpha)/2}\rangle \longrightarrow m(\varphi) = \begin{cases} 
1, & 0 \leq |\varphi| < \pi, \\
-1, & \text{otherwise},
\end{cases}
$$

$$
|\varphi^{N/2}\rangle |\varphi^{(1-\alpha)/2}\rangle \longrightarrow m(\varphi) = \begin{cases} 
1, & 0 \leq |\varphi| < \pi, \\
-1, & \text{otherwise},
\end{cases}
$$

$$
|\{\uparrow\downarrow\}^{N/2}\rangle \longrightarrow m(\varphi) = 0,
$$

$$
|\{\uparrow^2\downarrow\}^{N/3}\rangle \longrightarrow m(\varphi) = -1/3,
$$

$$
|\{\downarrow^2\uparrow\}^{N/6}\rangle |\{\uparrow^2\downarrow\}^{N/6}\rangle \longrightarrow m(\varphi) = \begin{cases} 
-1/3, & -\pi < \varphi < 0, \\
1/3, & \text{otherwise}.
\end{cases}
$$

(5.3)

We only wrote down for simplicity states with a step-wise characteristic function, but with little fantasy it is easy to imagine states with a smooth one.

---

1If we would be pedantic in defining this limit, we can think to $(1 + m(\varphi))/2$ as the convolution of the characteristic function of $E_x$ with a Gaussian of zero mean and standard deviation that must be put to zero at the end of any computation. Since in the sum in Eq. (5.3) there is almost everywhere (everywhere in non-critical regions) a regular function of $\varphi$, the regularization in the definition of $m(\varphi)$ is perfectly well-defined.
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5.1.1 The reduced density matrix and the entanglement entropy

We have seen that, despite the non-local character of the Jordan-Wigner transformation, the spectrum of the reduced density matrix $\rho_A$ of a single interval $A = [0, \ell]$ is the same in the spin variables $\sigma_l$ and in the free-fermion ones $c_l$ (cf. Eq. (2.117) and discussion below). This property makes the XY model the ideal testing-ground to understand the behavior of the single-block entanglement for excited states. In particular, the eigenvalues of the reduced density matrix $\rho_\ell$ of a block of $\ell$ adjacent spins for a Slater determinant are related to the eigenvalues $\nu_i$ of the correlation matrix restricted to the subsystem (cf. Eq. (2.108)). The two-by-two blocks of the correlation matrix $\Gamma_l$ defined in Eq. (2.34) are easily computed observing that the generic eigenstate in the Slater-determinant basis (5.1) is the vacuum of the fermionic operators

$$\hat{b}_k^\dagger = \begin{cases} b_k, & k \in E_x, \\ b_k^\dagger, & \text{otherwise.} \end{cases}$$

(5.4)

After simple algebra one obtains

$$\Gamma_l(E_x) = \Gamma_l^{(GS)} + \frac{2i}{L} \sum_{k \in E_x} \begin{pmatrix} \sin(l\varphi_k) & -\cos(l\varphi_k - \theta_k) \\ \cos(l\varphi_k + \theta_k) & \sin(l\varphi_k) \end{pmatrix},$$

(5.5)

where $\theta_k$ is the Bogoliubov angle of the transformation that diagonalizes the Hamiltonian in Eq. (2.29) and $\Gamma_l^{(GS)}$ the corresponding matrix in the ground state (cf. Eq. (2.34)).

As explained in the previous subsection, when $|E_x| \sim L$, we can substitute in equation (5.5) the sum with an integral

$$\frac{1}{L} \sum_{k \in E_x} \rightarrow \frac{1}{2\pi} \int_{-\pi}^{\pi} d\varphi \frac{1 + m(\varphi)}{2} \varphi_k \rightarrow \varphi,$$

(5.6)

where $(1 + m(\varphi))/2$ is the regularized characteristic function of the set $E_x$ introduced above. Substituting in Eq. (5.5) this regularization we have

$$\Gamma_l^{(E_x)} = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\varphi e^{-l\varphi} \Gamma_l^{(E_x)}, \quad \text{with}$$

$$\Gamma_\varphi^{(E_x)} = \frac{1}{2} \begin{pmatrix} m(-\varphi) - m(\varphi) & -i[m(\varphi) + m(-\varphi)]e^{-i\theta} \\ i[m(\varphi) + m(-\varphi)]e^{-i\theta} & m(-\varphi) - m(\varphi) \end{pmatrix}.$$ 

(5.7)

The entanglement entropy can be expressed as a complex integration over a contour $C$ that encircles the segment $[-1, 1]$ at the infinitesimal distance $\eta$ as in Ref. [23]

$$S_\ell = \lim_{\eta \rightarrow 0^+} \frac{1}{4\pi i} \oint_C d\lambda e(1 + 2\eta, \lambda) \frac{d}{d\lambda} \log \det |\lambda 1 - \Pi|,$$

(5.8)

where

$$e(x, y) = -\frac{x + y}{2} \log \frac{x + y}{2} - \frac{x - y}{2} \log \frac{x - y}{2}.$$
A similar expression is easily written for all Rényi entropies for general $\alpha$. Applying the Szégo lemma to the determinant of the block Toeplitz matrix $\lambda \mathbf{I} - \Pi$, we obtain the leading order in $\ell$ of the entanglement entropy

$$ S_\ell = \frac{\ell}{2\pi} \int_{-\pi}^{\pi} d\varphi \, H(m(\varphi)) + O(\log \ell), $$

with $H(x) = e(1, x)$. The entanglement entropy of a class of excited states in the XY model is extensive, in contrast with the logarithmic behavior of the ground state. However, every time that $m(\varphi)^2 \neq 1$ only in a region of vanishing measure of the domain (as in the ground state) this leading term vanishes, and one should go beyond the Szégo lemma to derive the first non-vanishing order of the entanglement entropy. It is important to stress that for this type of “highly excited states” the leading order of the entanglement entropy is not sensitive of the criticality of the ground state. This does not come unexpected, because we are exploring a region of energy that lies extensively above the ground state.

To describe the (subleading) logarithmic terms in the determinant of a Toeplitz matrix, we should use the Fisher-Hartwig conjecture \[79\]. If $m(\varphi)^2 = 1$ almost everywhere, $m(\varphi)$ can be re-written in the following form, that is particularly useful to apply Fisher-Hartwig ($\varphi \in [-\pi, \pi]$)

$$ m(\varphi) = e^{i \arg m(\pi)} \prod_{j=1}^{n} e^{i \arg (\varphi - \varphi_j)}, $$

where $2\lceil n/2 \rceil$ is the number of the discontinuities of $m(\varphi)$ and $\varphi_j$ are the discontinuity points (the term $2\lceil n/2 \rceil$ takes into account an eventual discontinuity in $\pi$ that is not counted by considering the open interval $\varphi \in (-\pi, \pi]$). We prove analytically in the next subsection that $S_\ell \propto \log \ell$ in the XX chain ($\gamma = 0$) and then we show that this is not a peculiar feature of the isotropic model.

### 5.1.2 XX chain

In the XX spin chain the Bogolioubov angle reduces to $e^{i \theta_k} = \text{sign}(J \cos \varphi_k - h)$ and the Fisher-Hartwig conjecture is sufficient to prove the following result: the entanglement entropy of the excited states described by the multi-step function \[5.10\] grows logarithmically with the width of the block. The coefficient in front of the logarithm is $1/6$ times the number of discontinuities in the non-critical region ($|h| > 1$) and it must be corrected in the critical region ($|h| < 1$) to take into account the modes with zero energy. For $|h| < 1$ the modes with zero energy at $\pm \varphi_F$ ($\varphi_F = \arccos |h/J|$) define the function

$$ \tilde{m}(\varphi) = \begin{cases} m(\varphi), & \varphi \in [\varphi_F, \varphi_F], \\ -m(-\varphi), & \text{otherwise}, \end{cases} $$

that substitutes $m(\varphi)$ when counting discontinuities. In Fig. 5.1 a direct computation shows the importance of the position of the modes with zero energy.
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Figure 5.1: Excited states of the XX model - The entanglement entropy as a function of the block length for the excited state with characteristic function \( m(\varphi) = \text{sign}(\varphi - \pi/6)(\pi/4 - \varphi) \) of two critical XX chains. The different behavior is caused by the position of the zero modes \( \varphi_F = \pi/6 \) and \( \pi/2 \) with two and four discontinuities respectively) and results in \( a = 1 \) or 2. The straight lines are the analytic prediction for large \( \ell \) given by Eqs. (5.17) and (5.18).

5.1.2.1 Proof of the log-behavior in the XX chain

The proof of the relation between the entanglement entropy and the discontinuities of \( m(\varphi) \) when Eq. (5.10) holds (i.e. when \( m(\varphi) = \pm 1 \)) in an XX chain is a slight modification of the proof given by Jin and Korepin in Ref. [23] for a critical XX ground state (see Chapter 4). For \( \gamma = 0 \), the matrix (5.7) can be written in terms of the Pauli matrix \( \sigma_y \) as

\[
\Gamma(\varphi) = \pm \sigma_y m(\mp \sigma_y \varphi),
\]

with the upper (lower) sign if the momentum \( \varphi \) is below (above) the Fermi level of the Jordan-Wigner fermions. As a consequence the block Toeplitz matrix can be reduced to a standard Toeplitz matrix with symbol

\[
\gamma(\varphi) = \begin{cases} 
1, & (e_\varphi > 0 \land m(-\varphi) = 1) \lor (e_\varphi < 0 \land m(\varphi) = -1), \\
-1, & \text{otherwise},
\end{cases}
\]

with \( e_\varphi = J \cos \varphi - h \). The reduced correlations matrix \( \lambda \mathbf{1} - \Pi \) is generated by the symbol

\[
t(\varphi) = \lambda - \prod_{j=1}^{n} e^{i \arg[\omega - \varphi_j]},
\]

where the \( \varphi_j \)'s are the momenta corresponding to the \( n \) discontinuities of \( \gamma(\varphi) \). The ground state has two symmetric discontinuities at \( \pm \varphi_F \). The symbol admits the canonical Fisher-Hartwig
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factorization \[79\]

\[ t(\varphi) = (\lambda + 1)^a(\lambda - 1)^b \prod_{j=1}^n t_j(\varphi), \]

with

\[ t_j(\varphi) = e^{-i\beta_j(\pi-\varphi_j)} \quad \varphi_j < \varphi < \varphi_j + 2\pi, \quad (5.14) \]

\[ \beta_j(\lambda) = \frac{(-1)^{j-1}}{2\pi i} \log \frac{\lambda + 1}{\lambda - 1}, \quad -\pi \leq \arg \left[ \frac{\lambda + 1}{\lambda - 1} \right] < \pi, \quad (5.15) \]

and the two exponents are

\[ b = 1 - a = \frac{1}{2\pi} \sum_{j=1}^n (-1)^{j-1} \varphi_j. \]

Defining \( k_F \equiv \sum_{j=1}^n (-1)^{j-1} \varphi_j / 2 \), the Fisher-Hartwig conjecture (that for this case with \(|\lambda| > 1\), i.e. \(|\text{Re}(\beta_j)| < 1/2\), has been proved by Basor \[80\]) reads as

\[ \det |\lambda I - \Pi| \sim \prod_{i<j}^n \left[ (2 - 2 \cos(\varphi_i - \varphi_j))^{(-1)^{i-j} \beta(\lambda)^2} \times G(1 + \beta(\lambda))^n G(1 - \beta(\lambda))^n \left( (\lambda + 1) \left( \frac{\lambda + 1}{\lambda - 1} \right)^{-k_F/\pi} \right)^{L-n\beta(\lambda)^2} \right], \quad (5.16) \]

where \( \beta^2 = \beta_j^2 \) and \( G(x) \) is the Barnes G-function

\[ G(1 + \beta)^n G(1 - \beta)^n = e^{-(1+\gamma n)\beta^2} \prod_{j=1}^\infty \left( 1 - \beta^2/j^2 \right)^j e^{jn\beta^2/j}. \]

In order to find the entanglement entropy we have to evaluate \( \frac{d}{d\lambda} \log D_\ell(\lambda) \), where \( D_\ell(\lambda) = \det |\lambda I - \Pi| \) (cf. Eq. (5.8)). The derivative can be easily computed and it consists (in principle) of three terms

\[ S_\ell = a_0 \ell + \frac{a}{3} \log \ell + a_{\{\varphi\}}, \quad (5.17) \]

with:

- the linear term \( a_0 \ell \) is the same as in the ground state \[23\] (except from the definition of \( k_F \)), and it is known to vanish \( a_0 = 0 \) (as actually we already proved);

- the logarithmic term \( a/3 \log \ell \) is the ground state contribution multiplied by \( a = n/2 \) (a will be interpreted as an effective central charge, that is why we multiplied by 1/3);

- the additive constant \( a_{\{\varphi\}} \) is slightly more complicated but it has essentially the same structure of the ground-state one:

\[ a_{\{\varphi\}} = \frac{n}{2} a_0 - \sum_{i<j}^n \frac{(-1)^{i-j}}{6} \log \left[ \sin^2 \left( \frac{\varphi_i - \varphi_j}{2} \right) \right], \quad (5.18) \]

with \( a_0 \) the additive constant for the entanglement entropy of the critical XX chain without magnetic field \( a_0 \approx 0.726 \ldots \) (see Ref. \[23\] for the analytic expression). Notice that it depends not only on the number of discontinuities but also on their location.
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See Fig. 5.1 for a comparison between this analytic asymptotic result and the direct computation for finite \( \ell \).

At this point it is natural to wonder whether these eigenstates, having an entanglement entropy growing logarithmically with \( \ell \), are the ground states of some conformal Hamiltonians. In the case of the XX model, since \( H_{XX}(h) \) with different magnetic fields commute among each other, the ground-state at given \( h \) is an excited state of a chain at different \( h \). Thus, for all these states it is obvious that they should display an entanglement entropy scaling like Eqs. (1.56) and (1.59) with \( c = a = 1 \), i.e. they have two discontinuities in \( \tilde{m}(\varphi) \). As we will see, this is true in general and in the next subsection we show that a commuting set of local operators of the XY chain can be used to prove that all these logarithmic excited states are ground states of properly defined local conformal Hamiltonians. Eq. (5.17) can be exploited to deduce the central charge of this local Hamiltonian \( c = a = n/2 \).

![Figure 5.2: Excited states of the XY model](image)

5.1.3 Logarithmic behavior and effective Hamiltonians

It is straightforward from Eq. (5.5) to calculate the spectrum of the reduced density matrix and the entanglement entropy for any eigenstate at any value of \( \gamma \) and \( h \). In fact, the entanglement entropy has a logarithmic behavior with \( \ell \) every time \( m(\varphi)^2 = 1 \) almost everywhere (see e.g. Fig. 5.2). This suggests that this type of excited states can be the ground states of critical Hamiltonians. We explicitly build these critical, translational invariant, and local Hamiltonians, proving the logarithmic behavior, with the correct prefactor.

The excited state \( |E_x\rangle \) in Eq. (5.1) is the ground state of all free-fermionic Hamiltonians of the form

\[
\tilde{H} = \sum_k \tilde{\varepsilon}(\varphi_k) b_k^\dagger b_k, \quad \text{with } \tilde{\varepsilon}(\varphi_k) < 0 \iff k \in E_x, \quad (5.19)
\]
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for any choice of the function $\tilde{\varepsilon}(\varphi_k)$. In particular we could choose $\tilde{\varepsilon}(\varphi_k) = -f(\varphi_k)m(\varphi_k)$, with $f(r)$ an arbitrary positive function. The choice of $\tilde{\varepsilon}(\varphi_k)$ determines the locality properties of $\hat{H}$: most of the choices of $\tilde{\varepsilon}(\varphi_k)$ would produce a non-local $\hat{H}$ (while by construction $\hat{H}$ is always hermitian and translational invariant because it is built by Fourier transform).

To understand the locality of this effective Hamiltonian it is useful to introduce the operators

$$G(r) = i \sum_{l} a_{l}^{x} a_{l+r}^{x}, \quad \text{and} \quad F^{x}(y)(r) = i \sum_{l} a_{l}^{x} a_{l+r}^{x}(y),$$

where $a_{l}^{x,y}$ are the Majorana operators defined in Eq. (2.35). In fact, by separating $\tilde{\varepsilon}(\varphi_k)$ in its even and odd part ($\tilde{\varepsilon}(\varphi_k) = \tilde{\varepsilon}_{e}(\varphi_k) + \tilde{\varepsilon}_{o}(\varphi_k)$), we can rewrite the effective Hamiltonian as the sum $\hat{H} = H_{e} + H_{o}$ where

$$H_{e} = \sum_{r} \left[ \frac{1}{N} \sum_{k=\frac{l}{N}}^{N-1} \tilde{\varepsilon}_{e}(\varphi_k)e^{i\theta_k}e^{-i\varphi r} \right] G_{r} \equiv \sum_{r} g_{e}(r) G_{r},$$

$$H_{o} = i \sum_{r} \left[ \frac{1}{2N} \sum_{k=\frac{l}{N}}^{N-1} \tilde{\varepsilon}_{o}(\varphi_k)e^{-i\varphi r} \right] \left( F^{x}_{r} + F^{y}_{r} \right) \equiv \sum_{r} g_{o}(r) (F^{x}_{r} + F^{y}_{r}),$$

where we defined the complex couplings $g_{e}(r)$ and $g_{o}(r)$.

The locality of $\hat{H}$ is related to the long distance behavior of these complex couplings $g_{e/o}(r)$. From a standard theorem in complex analysis, we know that $g_{e/o}(r)$ decays faster than any power (and so it results in local couplings) if its Fourier transform is $C^{\infty}$ (i.e. with all derivatives being continuous functions; often we will refer to these functions simply as regular). When Eq. (5.10) holds, that is $m(\varphi) = \pm 1$ has a finite number of discontinuities, and for a non-critical system (i.e. when $e^{-i\theta_k}$ is regular), the arbitrariness in the choice of $\tilde{\varepsilon}$ allows us to take it among the $C^{\infty}$ functions. This conclude the proof for non-critical systems.

For the critical case, a slight modification is enough to give the correct Hamiltonian. In the XX spin chain $e^{-i\varphi} = \text{sign}(J \cos \varphi - h)$ so that we can make the two above functions regular simply defining the characteristic function $\tilde{m}(\varphi)$

$$\tilde{m}(\varphi) = \begin{cases} m(\varphi) & \varphi \in [-\varphi, \varphi], \\ -m(-\varphi) & \text{otherwise}, \end{cases}$$

as we have already done in Eq. (5.11). The critical XY ($|h| = 1$) is more involved because $e^{-i\varphi}$ can be made regular only after imposing anti-periodic conditions to the mode of zero energy. It is then convenient to extend the definition of $\tilde{\varepsilon}$ to the interval $[0, 4\pi]$

$$\tilde{\varepsilon}_{(4\pi)}(\varphi) = \begin{cases} \tilde{\varepsilon}(\varphi) & \varphi \in [0, 2\pi] \\ -\tilde{\varepsilon}(4\pi - \varphi) & \varphi \in [2\pi, 4\pi]. \end{cases}$$

$\tilde{\varepsilon}_{(4\pi)}$ can be chosen $C^{\infty}$ because it has at most $2n + 2$ zeros, where $n$ is the number of the discontinuities corresponding to the excited state. The constructed function restricted to $[0, 2\pi]$
has the correct regularity properties. Regardless of the presence of a discontinuity in $\varphi = 0$ the dispersion law must vanish in $\varphi = 0$ (see Eq. (5.22)), thus the number of chiral modes is the number of discontinuities, plus 1 if there is not a discontinuity in $\varphi = 0$. This ends the construction of the local Hamiltonian for all the XY models. And this is not yet the end of the story. We can in fact use the arbitrariness we have in the choice of $\tilde{\varepsilon}_k$ to fix it in such a way that it crosses the zero-energy line with a non-vanishing slope. The low-energy properties of the resulting Hamiltonian can be then studied by linearizing the dispersion relation close to the zeros in a canonical manner. Each zero gives a chiral mode with central charge $1/2$ and so the total central charge will be $n/2$, with $n$ the number of zeros, i.e. the number of discontinuities of $m(\varphi)$ for non-critical systems, or the proper variation for critical ones (when the zero mode gives one additional contribution). This agrees with all the specific cases in the previous section. In particular if $m(\varphi)$ is discontinuous in $\varphi = 0$, the zero mode contributes only once. In Fig. 5.2 we report some specific examples stressing the importance of the critical modes and of the location of discontinuities.

### 5.1.4 Finite size scaling

When the width of the block $\ell$ is comparable with the length of the chain $L$, the characterization of the entanglement becomes tricky. When an excited state $|E_x\rangle$ can be associated to the ground-state of a local Hamiltonian $\tilde{H}$ with central charge $a = n/2$, i.e. when the entropy grows logarithmically with $\ell$ with a prefactor given by $a$, the constructive proof of previous subsection in the thermodynamic limit is still valid. Thus, in this case, the entanglement entropy has the finite size scaling given by Eq. (1.59) with $c$ replaced by $a$. This is shown in the right panel of Fig. 5.2.

A more intriguing problem is to understand the finite size scaling of excited states that have an extensive entanglement entropy in the thermodynamic limit. The result for $L \to \infty$ only predicts the derivative of the entropy for small subsystems. Increasing $\ell$ peculiar finite size behaviors must emerge, because the chain is finite and the entropy must be symmetric around $\ell = L/2$.

Up to now we studied in detail excited states with a regularized characteristic function of the type (5.10), that is $|E_x\rangle = |\prod_{j=1}^d \uparrow^{n_j} \downarrow^{m_j}\rangle$, where $n_j$ and $m_j$ are all $O(L)$ and $d$ is a finite number. States with $m(\varphi)^2 \neq 1$ (that have extensive entanglement entropy) do not fall in this category as evident in the definition (5.3). They can be realized by joining in a regular fashion small blocks $\kappa$ made up of a given sequence of populated or empty energy levels (e.g. $\kappa = \{\uparrow\}$ or $\kappa = \{\downarrow\}$ etc.). Thus, to study the finite size scaling of “extensive” states, we concentrate on those of the form

$$|E_x\rangle = |\prod_{j=1}^d \kappa^{n_j} \bar{\kappa}^{m_j}\rangle, \quad (5.23)$$

where $\bar{\kappa}$ is the set obtained interchanging $\uparrow$ with $\downarrow$. The entanglement entropy of this type of states in the thermodynamic limit has an extensive behavior because $\kappa$ averages to give
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Figure 5.3: \textit{n-folded wrapped chains} - Two 5-folded wrapped chains of 60 spins. The thick green line represents the subsystem (6 spins on the left and 18 spins on the right) while the red links give weight to the interaction between the subsystem and the rest of the chain. If the "area law" holds the entanglement entropy is proportional to the number of the links.

$m(\varphi) = (u - d)/(u + d)$, where $u$ ($d$) is the number of up (down) arrows in $\kappa$, while $\bar{\kappa}$ gives $m(\varphi) = (d - u)/(u + d)$: the regularized characteristic function is a multi-step function but with modulus different from 1. Eq. (5.9) gives the leading term of the entanglement entropy.

In order to have a quantitative prediction for the finite size scaling, we follow the ideas in the previous subsection by looking at the effective Hamiltonian obtained by the construction in Eq. (5.19). The resulting couplings in Eq. (5.20) could never give a finite-range Hamiltonian because the entanglement entropy is not logarithmic. We can make a local choice of the sign that makes $\bar{\varepsilon}$ a regular function (that we call $\bar{\varepsilon}$) giving the coupling

$$g(r) \equiv \frac{1}{L} \sum_{k=1}^{L-1} e^{ir\varphi_k} \bar{\varepsilon}(\varphi_k) = \frac{1}{L} \sum_{\varphi \in \mathbb{Z}} e^{-i|\kappa|kr\varphi} \left[ \bar{\varepsilon}(|\kappa|\varphi) + O(L^{-1}) \right] \sum_{n=1}^{|\kappa|} \kappa_n e^{-in\varphi}$$

and the interaction is not local anymore. The $O(1/L)$ term comes from the series expansion of $\bar{\varepsilon}$. The first factor in equation (5.24) is periodic of period $L/|\kappa|$ while the second one is a modulation. The coupling decays faster than any power for $r < L/2|\kappa|$, but it explodes (i.e. it grows faster than a power) up to $L/|\kappa|$ when $g(r)$ becomes again of order 1. The behavior for large distances is determined only by the first region

$$g(\frac{r + jL}{|\kappa|}) \approx \sum_{n=1}^{|\kappa|} \kappa_n \frac{e^{-i2\pi n\frac{r}{|\kappa|}} e^{-in\varphi}}{\sum_{n=1}^{|\kappa|} \kappa_n e^{-in\varphi}} g(r), \quad 0 < r < \frac{L}{|\kappa|}.$$  

\footnote{This coupling is a slight modification of the ones in Eq. (5.20). It has the advantage to make all the formulae simpler, but it applies only to non-critical systems. However all results (except for the ground state) are independent of this choice, as in the previous section.}
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The interaction is localized within a distance $jL/|\kappa|$, so the Hamiltonian can be interpreted as a local one in a $|\kappa|$-folded wrapped 1D chain. If we assume the “area law” to be valid for the wrapped chain (i.e. that only a shell of mutually interacting spins contributes to the entanglement [59]), we can predict the behavior of the entanglement entropy: each spin strongly interacts with the neighboring spins and with the $|\kappa|$ spins of the other wrappings (see Figure 5.3). Thus the entanglement entropy is a piece-wise function of $\ell$ that changes slope at $jL/|\kappa|$.

We can find excited states with analogous properties considering any finite partition of unity of the circle $]-\pi,\pi]$, with the property that all functions of the set are regular and approach step functions in the limit of large $L$. We associate a small block $\kappa^{(i)}$ to each function of the set and we write the coupling as a sum of terms of the form (5.24)

$$g(r) = \sum_{i=1}^{n} g_{\kappa^{(i)}}(r)$$

that we obtain identifying the regularized $\bar{\varepsilon}$ with the given function of the partition. In the scaling limit the characteristic function is $m \sim \prod_{i=1}^{n} \kappa_{(i)}^{(i)}$. Each $g_{\kappa^{(i)}}$ has the behavior previously described, so the entanglement entropy is a piece-wise function of $\ell$ changing slope in $jL/|\kappa|$, where $|\kappa|$ is the least common multiple of the $\{|\kappa|^{(i)}\}$. Two examples of 3-folded and 4-folded states are reported in Fig. 5.4.

![Figure 5.4: Examples of 3- and 4-folded states](image)

To give the details of a specific example, we report the 3-folded case $\kappa^{(1)} = \{\uparrow\downarrow\} = \{\uparrow\downarrow\}$ and $\kappa^{(0)} = \{\downarrow\}$ with $\varphi \in I_1 \iff \cos \varphi \geq 1/2$ and $\varphi \in I_0 \iff \cos \varphi < 1/2$, in other words the set $E_x$ is made of the quasiparticles with momenta $(2\pi(3k + q))/L$ with $|k| \leq L/12$ and $q \in \{0, 1\}$

$$|E_x\rangle = \prod_{k=-L/12}^{L/12} b_{3k+1}^\dagger b_{3k}^\dagger |0\rangle.$$
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The excited state $|E_x\rangle$ is the ground state of the Hamiltonian

$$\tilde{H} = \sum_{k=1}^{L-1} \left[ \left( \frac{1}{2} - \cos \varphi_k \right) (-1)^{\left\lfloor \frac{4k}{3} \right\rfloor} + (-1)^{\left\lfloor \frac{4k+1}{3} \right\rfloor} + (-1)^{\left\lfloor \frac{4k+2}{3} \right\rfloor} \right] b_k^\dagger b_k,$$

and if $L$ is divisible by 3 the coupling is different from 0 only in 9 points

$$g(r) = \begin{cases} \frac{5}{6} & r = 0, \\ -\frac{1}{6} & r = \pm 1, \\ -\frac{1}{6} \pm \frac{1}{\sqrt{12}} i & r = \pm \frac{L+q}{3}, \quad q \in \{-1, 0, 1\}. \end{cases}$$

The effective Hamiltonian $\tilde{H}$ is local on the 3-folded wrapped chain. The entropy grows linearly with the width of the block up to $\ell = L/3$, after that the interaction surface does not further increase and the entanglement entropy does not depend anymore on the width of the block, see Figure 5.4 (left). Notice on the same figure (right), the change of slope in the 4-folded case.

Figure 5.5: Half-chain entanglement entropy - Rescaled half-chain entanglement entropy $\ell = (L - 1)/2$ for a critical XX in zero magnetic field, a critical Ising, a non critical XY spin chain, and an Ising in a very large magnetic field. All plots are for $L = 15$. Each point corresponds to an excited state. The red curves are the “2-folded” estimations of the envelope.
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Figure 5.6: Quantization of half-chain entanglement entropy - Histograms for the number of the states with a given entanglement entropy for a non-critical XY chain of 23 spins, after cutting the Hilbert space in an energy shell. Main plot: rescaled $S_{11}$. Inset: rescaled $S_6$. The band-structure is evident only for $\ell = 11$.

5.1.5 Some general properties

To have a general picture of the scaling of the entanglement for all excited states and not only in the particular classes considered so far, we study here the entanglement entropy in a small enough chain to be able to calculate it for all the $2^L$ states. We mainly concentrate on blocks with maximal entropy, i.e. with length equal to half-chain (actually $(L - 1)/2$ spin, because we use $L$ odd). Drawing general conclusions in an analytic manner for finite systems is not easy, so we mainly analyze numerical results. The plots in Fig. 5.5 suggest that some regularities are general features of excited states and not only of the classes we can compute analytically. In these plots (and in all those relative to this section) we always consider the rescaled entropy

\[
\text{rescaled entropy} = \frac{S_\ell}{S_{\ell}^{GS}}, \quad \text{with} \quad S_{\ell}^{GS} = \frac{1}{3} \log \left( \frac{L}{\pi} \sin \frac{\pi \ell}{L} \right), \quad (5.25)
\]

so that, for states with a critical-like behavior (for large enough $\ell$ and $L$) we have a direct estimation of the effective central charge. We found particular instructive to plot the (rescaled) entanglement entropy as function of the energy of the eigenstates. In Fig. 5.5 we considered chains of 15 spins and we plot the rescaled $S_7$ for all the $2^{15}$ eigenstates. Similar plots can be done as function of total momentum instead of the energy.

A first feature that is particularly evident from the plots is the band-like structure of the entanglement entropy (notice that this is independent of the use of the energy on the horizontal axis, any other conserved quantity would result in qualitative similar plots). This means that the entanglement entropy of excited states distributes at roughly integer (or half-integer for critical
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XY at $h = 1$) multiples of $S^G_\ell$. For states with a small number of discontinuities (compared to $L$), this phenomenon is clearly due to the quantization of the prefactor of the logarithm. However, in general this band structure cannot be so easily explained: the excited states with a logarithmic behavior are expected to be negligible in number compared to all the others. Increasing the number of discontinuities at fixed $L$, the crossover to extensive behavior takes place and eventually it deteriorates the bands. This last phenomenon is not evident in Fig. 5.5 because the band structure persists up to the maximum allowed number of discontinuities. The simplest explanation is that also extensive states should roughly be quantized but within a scale different from $S^G_\ell$, that in particular does not grow with $L$. To check this, we should increase $L$, but in doing so, the dimension of the Hilbert space grows exponentially and it becomes soon prohibitive to plot (and understand) so many points in an readable graph. For this reason we considered a non-critical chain of 23 spins, and to reduce the number of states, we limited to the states with energy in the interval $4.600 < E - E_0 < 4.694$. In Fig. 5.6 we report the distribution of the points. For $\ell = 11$, the band structure is evident and the points distribute in an almost Gaussian fashion around some discrete values of the entanglement entropy, but the distance between them becomes smaller than $S^G_\ell$, confirming that the origin of this phenomenon in the upper part of the band has nothing to do with logarithmic states. For $\ell = 6$ (inset of Fig. 5.6) the band structure disappears completely, confirming that most of the states are extensive. We checked that still increasing $L$, this scenario is consistent.

Another very interesting feature is that in all the plots, the entanglement entropy has a maximum value that seems to be a regular function of the energy. We argue that these envelopes have a characteristic dependence on the energy that in the scaling limit is determined by excited states with extensive behavior. We already derived the entanglement entropy for the excited states that are equivalent to the ground state of $n$-folded wrapped Hamiltonians. Eq. (5.9) characterizes the scaling regime, e.g. for the 2-folded case the entanglement entropy increases linearly up to $L/2$, while in the 3-folded it increases up to $L/3$ and then saturates. We have then for blocks of length $\ell/L \geq H(1/3)/(2H(0)) = 0.459 \ldots$ that the 2-folded case is more entangled than the 3-folded one. This suggests that the 2-folded states can explain the envelopes in Fig. 5.5 for $\ell = (L - 1)/2$ (Notice that the maximal entangled state, regardless of the energy, is always a 2-folded one). If this is true, the envelope is easily obtained: the problem is analogous to find the dependence of the particles density on the Fermi energy in a free Fermi system at zero temperature. Indeed using Eq. (5.9) and the asymptotic expression for the energy, the “2-folded approximation” of the envelope satisfies the parametric equations (valid for $E < 0$)

$$
\frac{S^{MAX}}{L} \sim \frac{\log 2}{4\pi} \int_{-\pi}^{\pi} d\varphi \ \theta(\mu - \varepsilon), \\
\frac{E}{L} \sim -\frac{1}{4\pi} \int_{-\pi}^{\pi} d\varphi \ \varepsilon \ \theta(\varepsilon - \mu).
$$

In Fig. 5.5 this analytical result is compared with the numerical data for a critical XX, a critical Ising and two non critical XY spin chains: the approximate envelope is in good agreement with
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the numerical data also for small chains. We also notice that \( \frac{dS^{MAX}}{dE} = \log \frac{2}{\mu} \) and so

\[
\frac{dS^{MAX}}{dE} \leq \frac{\log 2}{\Delta} = \left( \frac{dS^{(MAX)}}{dE} \right)_{G.S.},
\]

where \( \Delta \) is the gap in the dispersion law: if the system is critical then the “2-folded” approximation of the envelope has infinite derivative in \( E = E_{G.S.} \) (cf. Fig. 5.5).

In the opposite limit of small \( \ell \), the band structure is practically lost (see left panel of Fig. 5.7) and for most of the states Eq. (5.9) gives a good estimate of \( S_\ell \) so that we expect that the envelope can be determined maximizing the expression (5.9) at fixed energy. The maximization gives the thermal-like parametric equations

\[
\frac{S^{MAX}}{\ell} \sim \frac{1}{2\pi} \int_{-\pi}^{\pi} d\varphi \ H(\tanh(\beta \varepsilon)),
\]

\[
\frac{E}{L} \sim \frac{1}{4\pi} \int_{-\pi}^{\pi} d\varphi \ \varepsilon \ \tanh(\beta \varepsilon),
\]

(5.27)

and the loss of the band structure can be seen as a consequence of a “pure” extensive behavior of the entropy. Eq. (5.27), in the scaling limit, is always an upper bound for the entanglement entropy because entropy is a concave function of \( \ell \). In Fig. 5.7 (left) we compare this analytical curve with the data for \( L = 15 \) and \( \ell = 4 \) in a non-critical XY-chain.

Considering blocks of intermediate lengths the parametric equations (5.27) define a too high bound (see right of Fig. 5.7). At the same time the band structure starts emerging. We can improve our estimation considering a generalization of the “2-folded approximation” of the envelope: the “n-folded approximation” (that makes sense only for \( \ell \leq L/n \)). The maximal
entanglement entropy in the $n$-folded family of excited states is

$$
\frac{S_{\text{MAX}}}{L} \sim \frac{H(1 - \frac{2}{n})}{2n\pi} \int_{-\pi}^{\pi} d\varphi \theta(\mu - \varepsilon),
$$

$$
\frac{E}{L} \sim \frac{1}{2n\pi} \int_{-\pi}^{\pi} d\varphi \varepsilon(\theta(\mu - \varepsilon) - \frac{n}{2}).
$$

(5.28)

In Fig. [5.7](right) we report $S_5$ for a non-critical Ising chain of 15 spins (so the maximum allowed $n$ is 3). It is evident that, up to the point where it exists, the 3-folded curve is a good approximation of the actual envelope, while for larger values Eq. (5.27) works well.

All the plots in this subsection are relative to the Slater-determinant basis. In fact considering linear combinations of eigenstates with the same energies, these envelopes remain unchanged, while the band-structure disappears.

### 5.2 Beyond “non-interacting” models

#### Figure 5.8: XXZ spin chain - Entanglement entropy for the two- and four-spinon states with $\Delta = 10^{-5}, 0.1, 0.3, 0.5$. Left: Summary of all the states we considered (for space problems, the legend shows only states at $\Delta = 0.3$). Right: Independence of the leading term on the spinon polarization. We considered $S_{\text{TOT}}^{z} = 0, 1, 2$. The slope does not depend on the polarization. The bottom-red line is the ground-state at $\Delta = 0.3$.

We conclude this chapter with the spin-$\frac{1}{2}$ XXZ model, whose Hamiltonian is given by

$$
H_{\text{XXZ}} = \sum_{m=1}^{N} \left[ \sigma_m^x \sigma_{m+1}^x + \sigma_m^y \sigma_{m+1}^y + \Delta(\sigma_m^z \sigma_{m+1}^z - 1) \right],
$$

(5.29)

with periodic boundary conditions. The model is solvable by Bethe Ansatz for any real value of the anisotropy parameter $\Delta$ [90], but we only consider the antiferromagnetic critical regime $0 < \Delta \leq 1$ (the case $\Delta = 0$ is the XX model, while $\Delta = 1$ is the XXX model). Here we do not describe the Bethe Ansatz solution of the model. We just mention that the ground state
of the model can be interpreted as the spinon vacuum. Spinons are the elementary excitations of the model. They have spin 1/2 and obey semionic exclusion statistics (see e.g. \cite{91} for a simple introduction to these excitations). Excited states have a defined number of up-spinon and down-spinon. In \cite{10} we found that one can construct a quantity directly related to the spinon representation, analogous to the characteristic function that we introduced for the XY model. And we checked whether the conformal scaling \(a\) with an effective central charge is still valid for given excited states when we add the interaction \(\Delta\) to the XX chain considered in the previous section. The prediction for the XX is based on the discontinuities of \(\tilde{m}(\phi)\) (cf. Eq. (5.11)). In order to predict the result at \(\Delta \neq 0\) we exploited the mapping between the fermionic description and the spinonic one at \(\Delta = 0\): once we have the fermionic picture associated to the state, we have \(\tilde{m}(\phi)\) for \(\Delta = 0\).

The numerical complexity drastically increases in considering \(\Delta\) different from 0, and we only explored relatively small chains \(L = 24\) and subsystems with length \(\ell \leq 6\). Despite of these difficulties, our results indicate that the general picture outlined analysing the XY model applies also to the interacting XXZ chain. For example in Fig. 5.8 (left) we display some states in the two-spinon and four-spinon sectors. We choose these states in such a way that, in the limit \(\Delta \to 0\), the corresponding fermionic structure has two discontinuities. For example, the state that we indicate with \(\circ^{6+} \bullet^{2+} \circ^{11+} \circ^{5-}\) (see \cite{10} for further details) corresponds to the fermion representation \(|\downarrow_8 \uparrow_{11} \downarrow_5\rangle\), having two discontinuities in \(\tilde{m}(\varphi)\). For \(\Delta = 0\), we know from the previous section that all these states are described by Eq. (4.1) with effective central charge \(a = 1\), as in the ground state. Fig. 5.8 (left) provides a clear evidence that the asymptotic behavior of the entropy for \(\ell \gg 1\) does not depend on \(\Delta\), at least in the considered range \(\Delta \in [0, 0.5]\). In the figure we also report the ground-state value for \(\Delta = 0.3\) for comparison.

The fact that the division among extensive and logarithmic states is conserved when the interaction \(\Delta\) is introduced, strongly suggests that this phenomenon should be expected for any local spin chain, with a prefactor that can be predicted after that the relevant excitations have been identified. In fact, in the interacting system (especially for \(\Delta\) not small) the excited states are complicated linear combinations of the free-particle ones, several degenerations are also removed by \(\Delta\), and it is unlikely that such result is only a coincidence. However, we do not have a general proof for this statement.

In this chapter we reported some of the results obtained in Ref. \cite{10}, where we analyzed the excited states of the XY model and of the XXZ chain. We have chosen a basis independent of the dispersion relations of excitations and well-defined for any chain’s size, namely in the XY model the basis of Slater determinants. By analyzing the entanglement entropy of connected subsystems, two classes of excited states can be distinguished: states in which the entanglement entropy is extensive and states in which instead it behaves as in the ground state of critical
systems. In the following chapter we consider an example of system in which the criticality is not related to the symmetries of the Hamiltonian.
5. ENTANGLEMENT ENTROPY OF EXCITED STATES
6. Entanglement in quantum random systems

The ground state of a system at a quantum critical point shows universal behavior in many quantities. Correlation functions, for example, have universal power-law behavior, which, in some cases, can be obtained exactly by mapping the quantum critical point to a system in one more dimension. In the previous chapters we have provided many examples indicative of the power of this mapping for one-dimensional (1D) quantum critical points (QCPs) that become 2D classical critical points with conformal invariance. In addition to standard correlation functions, we have shown in the introductory chapter that the entanglement entropy is universal at such points, and determined by the central charge of the associated 2D conformal field theory [52].

Other properties related to entanglement are less well understood, such as the entanglement spectrum (the full set of reduced density matrix eigenvalues) and the full set of entanglement Renyi entropies; one exception is free Fermi models, where the entanglement spectrum is given by the spectrum of an effective “entanglement Hamiltonian” [73,92,93]. This is given by the quadratic form characterizing the RDM, i.e.

\[
\frac{1}{2} \sum_{ln} a_l \left[ \arctanh(\Gamma) \right]_l a_n \tag{6.1}
\]

where \( \Gamma \) is the correlation matrix (see Sec. 2.2). Notice however that the entanglement spectrum becomes inaccessible when the system is a “non-interacting” spin chain but the subsystem is not connected (cf. Chapter 3).

In this chapter we present the results obtained in Ref. [8] where we studied the entanglement spectrum at “random-singlet” 1D QCPs, in which quenched disorder leads to an RG flow to infinite randomness. We obtain the disorder-averaged moments of the Schmidt eigenvalue distribution analytically and compare them to numerical results on a special case with a free-fermion representation, the random XX model. While these critical points are not conformally invariant (after mapping to a 2D problem, the imaginary-time direction has no randomness and is hence very different from the spatial direction), their disorder-averaged correlation functions have nevertheless been understood in many cases [39] by real-space renormalization group method [40]. In Sec. 1.2.2 we have shown that the entanglement entropy at random-singlet
critical points has universal behavior similar to that at 1D conformal QCPs (cf. Eq. [1.57]), with a modified prefactor of the logarithm (analogous to $c$) that was initially viewed as an effective central charge for random systems.

However this similarity does not extend to the full entanglement spectra, which are rather different. We start by considering the disorder-averaged Renyi entropies

$$S_\alpha = \frac{1}{1 - \alpha} \ln \text{Tr} \rho_\alpha^A,$$

(6.2)

where the bar denotes the average over quenched disorder. These Renyi entropies $S_\alpha$ are quite simple in the random-singlet phase: they depend only on the mean number of singlets across the partition used to define the entanglement, just as does the entanglement entropy. The Renyi entropies already behave differently than in the conformal case. However, in disordered systems $S_\alpha$ is not the right quantity that determines the entanglement spectrum via Laplace transform in $\alpha$ [25]. To obtain the averaged moments of the distribution, one should instead consider the entropies corresponding to averaging the disorder before taking the logarithm

$$\tilde{S}_\alpha = \frac{1}{1 - \alpha} \ln \text{Tr} \rho_\alpha^A.$$

(6.3)

This definition has also the advantage to maintain the relationship of the pure system between the Tsallis [94] entropies $(\text{Tr} \rho_\alpha^A - 1)/(1 - \alpha)$ and the Renyi entropies. The moments of the entanglement eigenvalue distribution reveal the full distribution of the number of singlets crossing a boundary and require an improved calculation. Both generalized entropies reduce to the Von Neumann one as $\alpha$ approaches 1

$$S_{VN} = \lim_{\alpha \to 1} S_\alpha = \lim_{\alpha \to 1} \tilde{S}_\alpha.$$

(6.4)

6.1 Random-singlet picture of the Renyi entropies

In section 1.2.2 we studied the disorder-averaged Rényi entropies in the random singlet phase: they are equal and proportional to the number of in-out singlets

$$S^{RSP}_\alpha = \pi \ln 2.$$

(6.5)

After some manipulation (see Section 1.2.2), the averaged number of singlets in the disordered XX chain can be expressed in terms of the block’s length [42]

$$\pi \simeq \frac{1}{3} \ln \ell,$$

(6.6)

and so the entanglement entropy of a block of length $\ell$ is

$$S_{VN}^{RSP}(\ell) \simeq \frac{\ln 2}{3} \ln \ell,$$

(6.7)

with a weight-factor $\frac{\ln 2}{3}$ that calls to mind the behavior in the absence of disorder with an effective central charge $\ln 2$. 

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6.2 Generalized entropy and the probability distribution of singlet formation

Consideration of the R\'enyi entropy rather than the standard entanglement entropy suggests that the similarity between the entanglement entropy with and without disorder is only superficial. Indeed in the RSP all R\'enyi entropies scale in the same way [6.5]. If we wish to define an effective central charge, we could use any conformal R\'enyi entropy \[5\]

\[
S^{CFT}_\alpha(\ell) = \frac{c}{6} \left(1 + \frac{1}{\alpha}\right) \ln \frac{\ell}{a} + c'_\alpha, \tag{6.8}
\]
as starting point, so that the effective central charge would have any value in the range \([\ln 4^{-1}, (\ln 2)^{-1}]\) while \(\alpha\) runs from 1 to infinity. Also the central charge of the clean system \(c = 1\) belongs to this range, making questionable any attempt to generalize the Zamolodchikov “c-theorem” [95]. In fact, there is no version of the c-theorem for entanglement entropy that would describe the flow from clean to random systems [96][97] or within random systems [98].

The disorder-averaged R\'enyi entropies at random quantum critical points are universal and indicate that the random-singlet phase’s entanglement is quite different from the universal entanglement at 1D conformal QCPs. However, since they depend on the same quantity (mean number \(\bar{n}\) of in-out singlets) as the entanglement entropy, they do not probe new features of the random-singlet picture. In the next section we consider the quantities (6.3), which are sensitive to new features and directly probe a memory effect in the RSRG flow, or “repulsion between decimations” in RG space, that was a key step in obtaining the correct value of \(\bar{n}\). Numerical tests of the predicted R\'enyi entropies are described in Section [6.3].

6.2 Generalized entropy and the probability distribution of singlet formation

A natural measure of the full in-out singlet distribution \(P(n)\), or the probability distribution of the Reny entropy, can be examined by considering \(\hat{S}_\alpha\) in Eq. (6.3). In fact, denoting by \(g(t)\) the cumulant-generating function of the in-out singlet distribution \(P(n)\)

\[
g(t) = \ln \langle e^{nt} \rangle \equiv \ln \sum_{n=0}^{\infty} P(n) e^{nt}, \tag{6.9}
\]
it is straightforward that

\[
\hat{S}^{RSP}_\alpha = \frac{g(t(\alpha))}{1 - \alpha}, \tag{6.10}
\]
where, to keep the notation compact, we defined

\[
t = t(\alpha) \equiv (1 - \alpha) \ln 2. \tag{6.11}
\]
Through all this chapter \(t\) will always denote this quantity, even when the \(\alpha\) dependence is not specified. \(\hat{S}_\alpha\) does depend on \(\alpha\) in the RSP, unlike the R\'enyi entropy \(S_\alpha\). We require Eq. (6.9) to not blow up when \(n \to \infty\), and so (assuming a reasonable \(P(n)\)) we need \(t \leq 0\) corresponding to \(\alpha \geq 1\).
6. ENTANGLEMENT IN QUANTUM RANDOM SYSTEMS

From the real-space renormalization group (RSRG) point of view, singlets form at a constant rate with respect to an “RG time” $\mu$, and this rate determines the logarithmic scaling of entanglement entropy. En route to calculating this rate, Ref. [42] obtains the expression for the distribution of waiting times for a decimation across a bond since the last decimation:

$$f(\mu) = \frac{1}{\sqrt{5}} \left( e^{-\frac{3+\sqrt{5}}{2} \mu} - e^{-\frac{3-\sqrt{5}}{2} \mu} \right).$$

(6.12)

The above distribution has been deduced neglecting non-universal terms coming from the starting disorder distribution: Eq. (6.12) is only asymptotically true. For example, we expect that the additive constant of the von Neumann entropy $S_{VN}$ should be disorder dependent.

During the RG time between two decimations several processes can happen. The most probable one is the formation of isolated singlets. Considering only this process leads to the renewal equation (cf. Eq. (1.80))

$$\langle \text{ent} \rangle_\mu = \int_{\mu}^{\infty} d\mu' f(\mu') + e^t \int_{0}^{\mu} d\mu' f(\mu') \langle \text{ent} \rangle_{\mu'-\mu}. $$

(6.13)

This can be solved by Laplace transformation. Calling $\hat{f}(s)$ the Laplace transform of $f(\mu)$

$$\hat{g}(s) = \frac{1}{\sqrt{5}} \left( \frac{1}{s + \frac{3-\sqrt{5}}{2}} - \frac{1}{s + \frac{3+\sqrt{5}}{2}} \right),$$

(6.14)

we have

$$g(\mu)(t) = \ln \left[ Z^{-1} \left\{ \frac{1}{s} - \frac{1}{s - e^t \hat{f}(s)} \right\} (\mu) \right],$$

(6.15)

and in particular $\pi = \lim_{t \to 0} g'(t)$.

After simple algebra, we obtain

$$e^{g(\mu)(t)} = \left( \frac{1}{2} + \frac{3}{2\sqrt{5} + 4e^t} \right) e^{-\frac{3-\sqrt{5}}{2} \mu} + \left( \frac{1}{2} - \frac{3}{2\sqrt{5} + 4e^t} \right) e^{-\frac{3+\sqrt{5}}{2} \mu},$$

(6.16)

that via Eq. (6.10) gives $\tilde{S}_\alpha$ in the RSP. It is useful to rewrite it in terms of the mean number of singlets as

$$g(t) = tA_t \pi + tB_t,$$

(6.17)

where the multiplicative $t$ factor is introduced to write more compact formulae for $\tilde{S}_\alpha$ via Eq. (6.10). The two constants $A_t$ and $B_t$ are obtained by plugging (6.17) into (6.16):

$$A_t = 3\sqrt{5} + 4e^t - 3,$$

$$B_t = \frac{1}{6} \ln \left( \frac{1}{2} + \frac{3}{\sqrt{5} + 4e^t} \right) + \frac{\sqrt{5} + 4e^t - 3}{6t}.$$

(6.18)

Notice that in Eq. (6.17) all the dependence of $g(\mu)(t)$ on $\mu$ is encoded in $\pi$. In this way, we also separated the universal $\ln \ell$ behavior (we remind $\pi \propto \ln \ell$) given by $A_t$ from the constant one $B_t$. We will come back to the discussion of the universal features of Eqs. (6.17) and (6.18) in the next section when comparing with the numerical results.
6.3 Numerical Results

In this section we present the numerical results obtained in Ref. [8]. The entropies \( S_\alpha \) and \( \hat{S}_\alpha \) can be directly calculated for the disordered XX chain (2.15), by generalizing the method of Laflorencie [99]. In fact, for any realization of the disorder (i.e. any distribution of the bonds \( J_l \)), the XX model can be mapped into a free-fermionic Hamiltonian by the Jordan-Wigner transformation \( c_l^\dagger = \prod_{j<l} \sigma_j^z \sigma_j^x \), that leaves the eigenvalues of the reduced density matrix of a single block unchanged, being the transformation local inside of the block. Defining the correlation matrix \( C_{ln} = \langle c_l^\dagger c_n \rangle \), the reduced density matrix of a spin block that goes from the site \( l_0 + 1 \) to \( l_0 + \ell \) is the exponential of a free-fermion operator (cf. Eq. (2.103)) and it is completely characterized by the \( \ell \times \ell \) correlation matrix \( C_{l_0}^{[\ell]} \) in which indexes run from \( l_0 + 1 \) to \( l_0 + \ell \). The entanglement entropy of the block in this configuration of the disorder is then given by

\[
S_{VN}^{[l_0]}(\{J_l\}) = -\text{Tr}C_{l_0}^{[\ell]} \ln C_{l_0}^{[\ell]} + (1 - C_{l_0}^{[\ell]}) \ln(1 - C_{l_0}^{[\ell]}),
\]

(6.19)

while the Renyi entropy is

\[
S_{\alpha}^{[l_0]}(\{J_l\}) = \frac{1}{1-\alpha} \text{Tr} \ln \left((C_{l_0}^{[\ell]})^\alpha + (1 - C_{l_0}^{[\ell]})^\alpha\right),
\]

(6.20)

where we stressed the dependence on the disorder configuration (\( \{J_l\} \)) and on the first site of the block \( l_0 + 1 \). Indeed, on a single realization of the disorder, translational invariance is explicitly broken. Only after taking the disorder average, translational symmetry can be restored. Having the Renyi entropies for a single realization allows to obtain the asymptotic results for the disordered model by averaging over a large enough number of configurations (generated randomly according to the specific rules for \( \{J_l\} \)). \( S_\alpha \) and \( \hat{S}_\alpha \) are obtained by averaging \( S_\alpha \) or \( e^{(1-\alpha)S_\alpha} \), respectively.

The method is an ab-initio calculation of the Renyi entropies for disordered spin chains valid every time the model has a free-fermionic representation (as in XX or Ising chains). It is however numerically demanding. A more effective numerical technique exploits the RSP structure of the ground state. Starting from a given disorder realization, we construct a singlet where the strong bond lies and we proceed to decimation according to the Ma-Dasgupta rule in Eq. (1.68). We repeat this procedure until we spanned all the chain. At this point we are left with a collection of singlets, and then, counting number of singlets connecting the inside of the block with the outside, we have the configurational Renyi entropies from the relation \( S_\alpha^{[l_0]}(\{J_l\}) = n^{[l_0]} (\{J_l\}) \ln 2 \). As for the ab-initio calculation, \( S_\alpha \) and \( \hat{S}_\alpha \) are obtained by averaging over the disorder. Note that \( S_\alpha^{RSP} \) does not depend on \( \alpha \) by definition, since for any configuration \( S_\alpha = \pi \ln 2 \). Oppositely \( \hat{S}_\alpha \) depends on \( \alpha \) because the average is taken over \( e^{(1-\alpha)S_\alpha} \). For completeness, we give few general features for an intuitive picture of the entanglement in the RSP. After a decimation (1.68), the renormalized bond is strongly suppressed, i.e. singlets repel. The singlets that stay inside of the block involve always an even number of spins, thus the parity of the block gives the parity of the number of in-out singlets. The spins belonging
to the longest bonds crossing the two ends of the chain can be also thought as boundaries of two open chains. This suggests that in the RSP (as it is the case for clean systems [5]) the entanglement entropy of a block of \( \ell \) spins in a periodic chain is equivalent to twice the entanglement entropy of \( \ell/2 \) spins in an open chain with the block starting from the boundary, i.e. \( S_{\text{periodic}}(\ell) \approx 2S_{\text{open}}(\ell/2) \). However, this argument does not provide information about the additive constant (in clean models, the difference of the two constant terms gives the Affleck and Ludwig boundary entropy [75]).

To avoid confusion between the two determinations of the entanglement, in the following we will always refer to the first method as \textit{ab-initio} while to the second as RSP. We stress that the RSP technique can be applied to any model with an RSP ground state, as for example the disordered Heisenberg chains or spin-1 chains [43], while the ab-initio one only to models having a free-femionic representation. However, the ab-initio method has the advantage to be exact by definition. Instead, by counting the number of singlets, we make the assumption that the ground state has an RSP structure and that all the universal entanglement physics can be extracted from this. Although both assumptions sound reasonable, it is always worthwhile to perform in parallel the two numerical studies. In fact, the numerical counting of singlets is not the same as the analytic expressions derived in the previous sections because, in order to provide analytic results, few further assumptions have been made (e.g. considering only the formation of isolated singlets etc.). In case of disagreement between formulae and numerics, making the two computations in parallel helps to understand if the error is in the approximations made to solve the equations or in the RSP assumption itself.

### 6.3.1 Analysis of \( S_\alpha \)

We start analyzing the averaged R\'enyi entropies \( S_\alpha \) for many different system sizes. In Fig. 6.1 we report the result for a chain of \( L = 1024 \) spins for the disorder average over a sample of 73000 realizations. For \( 1 \ll \ell \ll L \), the various curves are parallel, with the slope predicted by Eq. (6.7), i.e. the leading term of \( S_\alpha \) is \( \alpha \) independent. The non-universal additive \( O(\ell^0) \) term clearly depends on \( \alpha \), as in the clean case. On top of a smooth behavior, we can see oscillating contributions, evident for small \( \ell \) and large \( \alpha \). Their presence does not come unexpected: we have already discussed in Chapter 4 the analogous oscillating terms that appear in clean systems. However, for random systems the oscillations have a different form and they decay rather quickly with \( \ell \) (as opposite to \( \hat{S}_\alpha \) as we shall see). When \( \ell \) approaches the chain length \( L \), sizable finite-size corrections are visible. Next subsection will be devoted to their accurate study, while here we continue with the asymptotic analysis of \( S_\alpha \).

We compare the data in Fig. 6.1 from the ab-initio calculation, with the numerical results obtained using the RSP approach on the same random sample of 73000 realizations of \( J_l \). According to Eq. (6.5), the RSP R\'enyi entropies do not depend on \( \alpha \) by definition. For this reason, in Fig. 6.2 we report the difference between the RSP R\'enyi entropies and the ab-initio ones presented in Fig. 6.1. After a transient behavior for small \( \ell \), all the curves with varying \( \alpha \)
6.3 Numerical Results

**Figure 6.1:** *Ab-initio* Rényi entropies - *Ab-initio* Rényi entropies for a disordered XX chain of 1024 spins. The average is over 73000 realizations. The variation of the color shows results from $\alpha = 1$ (upper line) to $\alpha = 2.9$ (bottom line). The yellow line is the asymptotic Von Neumann entropy ($\alpha = 1$) obtained by Laflorencie [99].

**Figure 6.2:** $S_\alpha - S^{RSP}$ - *Ab-initio* Rényi entropies for a disordered XX chain of 1024 spins minus the RSP value. The averages are over the same sample of 73000 realizations.
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approach a constant, indicating not only that the universal leading logarithmic term in $S_\alpha$ is correctly described by RSP, but also the finite size corrections are. In the range of $\alpha$ considered in the figure, we find that the additive constant is well described by

$$S_\alpha \approx S^{RSP}_\alpha + \frac{a}{\alpha} + b + o(1), \quad (6.21)$$

where the disorder-dependent constants $a$ and $b$ in the case of random disorder take the values $a \approx 0.61$ and $b \approx -0.47$.

6.3.2 Finite-size effects

Having established the correctness of the asymptotic RSRG results for $S_\alpha$ in the region $1 \ll \ell \ll L$, we can consider the finite-size effects. One of the most remarkable result of conformal invariance is that the finite-size scaling is obtained by replacing the subsystem’s length with the chord length

$$\ell \rightarrow \frac{L}{\pi} \sin\left(\frac{\pi \ell}{L}\right). \quad (6.22)$$

in the thermodynamic limit result. However, when conformal invariance is broken, the chord length does not give the finite-size scaling. In fact, using the results reported above, it is easy to show that this is the case, as it was shown before for some random Ising systems [100].

Even if conformal invariance is broken, scale invariance still holds. Thus the finite size

Figure 6.3: Finite-size scaling function - The finite-size scaling function for the entanglement entropy $Y(x)$ in Eq. (6.23). Main: RSP data averaged over 1440000 disorder realizations for $L = 1024$. The continuous (red) curve is the proposed phenomenological formula (6.25) describing perfectly the data points. Inset: The same plot for different values of $L$, showing the collapse on a single scaling function.
scaling can always be taken into account by the substitution
\[ \ell \rightarrow \frac{L}{\pi} Y \left( \frac{\pi \ell}{L} \right). \]

(6.23)

The great predictive power of conformal symmetry is that independently of the observable (but built with primary operators) the scaling function is always \( Y(x) = \sin(x) \), while in general scale-invariant theories the function \( Y(x) \) does depend on the observable. The function \( Y(x) \) for \( S_\alpha \) must however satisfy simple symmetry constraints. First, \( S_\alpha \) is symmetric for \( \ell \rightarrow L - \ell \), thus \( Y(x) = Y(\pi - x) \). Second, periodic boundary conditions require \( S_\alpha \) to be a periodic function of \( \ell \) of period \( L \), and so \( Y(x) = Y(\pi + x) \). Thus we can expand \( Y(x) \) in Fourier modes as
\[ Y(x) = \left[ 1 + \sum_{j=1}^{\infty} k_j \right] \sin x - \sum_{k=1}^{\infty} \frac{k_j}{2j + 1} \sin((2j + 1)x), \]

(6.24)

where we also imposed \( Y(x \ll 1) \sim x \) to reproduce the correct thermodynamic limit. The chord length has only the first mode and so corresponds to \( k_j = 0 \) for any \( j \). This expansion in terms of Fourier modes is particularly useful, because we expect that the contribution of the first few modes will be enough to have a reasonable approximation of the scaling function \( Y(x) \). Indeed, Fig. 6.3 shows that only the first term \( k_1 \) is enough to describe accurately the observed behavior for the RSP entanglement entropy
\[ Y(x) \simeq (1 + k_1) \sin x - \frac{k_1}{3} \sin 3x = \sin x \left[ 1 + \frac{4}{3} k_1 \sin^2 x \right], \]

(6.25)

with \( k_1 \approx 0.115 \). The obtained scaling function in presence of disorder is greater than the chord length.

Fig. 6.2 shows that the finite-size scaling in the ab-initio calculation are equivalent to the RSP ones (else for \( \ell \sim L \) the various curves should bend). This means that the finite-size scaling of all \( S_\alpha \) in the spin chain is described by Eq. (6.25), as we also checked directly.

6.3.3 Probability distribution of the R\'enyi entropy

To sum up, the disorder averaged R\'enyi entropy \( S_\alpha \) gives only access to the averaged number of the in-out singlets, while \( \hat{S}_\alpha \) gives access to the full in-out singlets distribution \( P(n) \), i.e. the probability distribution of the R\'enyi entropy and so to the full entanglement spectrum. Indeed \( \hat{S}_\alpha \) is related to the cumulant generating function \( g(t) \) of the in-out singlets distribution by Eq. (6.10).

We first consider the RSP data, because they allow to explore larger system sizes. Only after having established the asymptotic behavior we will consider ab-initio data and show consistency with the proposed scaling.

R\'enyi entropies \( S_\alpha^{RSP} \) do not have subleading corrections depending on the parity of the block, making the asymptotic analysis quite straightforward. Oppositely, the data for \( \hat{S}_\alpha^{RSP} \) (see Fig. 6.4) show that they depend on the block parity in a way similar to clean systems.
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Figure 6.4: $\hat{S}_\alpha$ - Top: RSP results for $\hat{S}_\alpha$ as a function of $S_\alpha$ for a chain of 1024 spins and 1440000 disorder realizations. Right: Even-odd average of $\hat{S}_\alpha$ eliminating leading corrections to the scaling. In both panels, the continuous lines are the analytic RSRG result for $A_t$.

To analyze the numerical data in Ref. [8] we have conjectured the following asymptotic behavior

$$\hat{S}_\alpha^{RSP}(\ell) \approx A_t S_\alpha^{RSP}(\ell) + B_t \ln 2 - (-1)^\ell f_t (S_\alpha^{RSP}(\ell)) \ln 2,$$

(6.26)

where $t$ is defined in Eq. (6.11). $A_t$ and $B_t$ are the two functions introduced in Eq. (6.17), while $f_t$ takes into account the corrections to the scaling and goes to 0 for $\ell \to \infty$. The form of the corrections is inspired by the results in clean systems, while the leading term is the asymptotic solution $g(t)$ in Eqs. (6.17) and (6.18). In the top of Fig. 6.4 we also report the RSRG value for $A_t$ that seems to be in qualitative agreement with the numerical data. A full quantitative description requires the elimination of the corrections to the scaling.

In order to provide an unbiased description of the asymptotic behavior of $\hat{S}_\alpha$, we define the functions $s_\alpha^{even}(\ell)$ and $s_\alpha^{odd}(\ell)$ from the interpolation relative to even and odd blocks respectively. We can isolate the leading behavior of $\hat{S}_\alpha^{RSP}$ by considering the average over the two interpolating functions, i.e.

$$\hat{S}_\alpha^{eo}(\ell) \equiv \frac{s_\alpha^{even}(\ell) + s_\alpha^{odd}(\ell)}{2}.$$

(6.27)

This definition eliminates the leading corrections to the scaling. In fact, in the right panel of Fig. 6.4 we have a linear relation between $\hat{S}_\alpha^{eo}$ and $S_\alpha^{RSP}$ for all reported values of $\alpha$ (while the non-averaged data in the left panel are linear only for $\alpha$ close to 1).

From this linear dependence we can extract the functions $A_t$ and $B_t$ using the RSRG relation

$$\hat{S}_\alpha^{eo} \approx A_t S_\alpha^{RSP}(\ell) + \ln 2 B_t.$$

(6.28)

The resulting values for the universal coefficient $A_t(\alpha)$ for $\alpha \leq 10$ and for $L = 1024$ and $L = 10000$ are reported in Fig. 6.5. For small $\alpha$ ($\leq 3.5$) there are negligible finite-size corrections and data perfectly agree with the RSRG result in Eq. (6.18), showing the predictive power of the RSRG to determine $A_t$. For larger $\alpha$, finite-size corrections are important and indeed data
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Figure 6.5: Universal proportionality factor - The universal constant $A_t$ obtained from RSP data for $L = 1024$ (1440000 disorder realizations) and $L = 10000$ (320000 realizations). Main plot: For $\alpha \leq 3.5$ finite-size effects are negligible and the RSRG prediction (continuous line) describes the data. Inset: Crossover to the non-universal Poissonian behavior (green continuous line) for larger $\alpha$.

differ from the analytical prediction, but the larger system sizes are closer. We believe that in the thermodynamic limit the RSRG $A_t$ describes the correct behavior for any $\alpha$. The reason of these finite-size effects is also easily understood: the asymptotic formula is valid for $\hat{S \alpha}$ large, while in this region of $\alpha$ we have $\hat{S \alpha} \sim 1$. Even if not asymptotic, the large $\alpha$ results show an interesting behavior: independently of $L$, they follow a $-1/t$ behavior (see inset in Fig. 6.5), typical of a Poissonian distribution of singlets. The reason of this Poissonian behavior can be traced back to the fact that for $t \to -\infty$ we are giving a large weight to short-range singlets that are produced almost independently. Little weight is instead given to long-range singlets responsible for the universal physics and so for these values of $\alpha$ and $L$ we are probing the UV physics. According to this interpretation, a crossover from the universal behavior of Eq. (6.18) to a UV Poissonian behavior always takes place for $\alpha \sim \ln L$, in agreement with Fig. 6.5.

We can now move to the ab-initio calculation to check the validity of the RSP scenario for $\hat{S \alpha}$. As before, we focus on the relation between $\hat{S \alpha}$ and $S \alpha$ and in particular on the universal slope of the linear relation between them. The results are reported in Fig. 6.6. Asymptotically, the slopes of these curves tend to the RSRG prediction for $A_t$ shown as continuous lines in the figure. Also the finite-size scaling is well described by Eq. (6.25), as evident from the fact that the linear relation between $\hat{S \alpha}$ and $S \alpha$ is correct even for large values of $t$ (i.e. of $S \alpha$) in the various plots. However, as clear by a visual comparison between Figs. 6.6 and 6.4 (left), the constant term in this relation is different (and both different from the analytic $B_t$ in Eq. 6.18).
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Figure 6.6: $\tilde{S}_\alpha$ vs $S_\alpha$ - Ab-initio $\tilde{S}_\alpha$ as a function of $S_\alpha$ for a spin-chain of 1024 spins and 73000 disorder realizations. The continuous lines represent the RSRG prediction for the slope. The additive terms are different from those in Fig. 6.4.

The degree of universality of this term is discussed in the next subsection.

Having established the correct asymptotic behavior we can consider the oscillating corrections to the scaling defined in Eq. (6.26). The numerical estimate of $f_t(S)$ can be obtained as

$$f_t(S) \simeq \frac{s^{\text{odd}}(\ell)}{2} - \frac{s^{\text{even}}(\ell)}{2} + \ldots,$$

(6.29)

where the dots denotes subsubleading terms (we recall $s^{\text{odd/even}}_\alpha$ are interpolations and so defined for any $\ell$). The data obtained in this way are reported in Fig. 6.7. The linear behavior in log-scale shows that for $\alpha \leq 5$ (for larger $\alpha$ further sub-leading corrections must be considered \[71\]) $f_t(S_\alpha)$ decays exponentially

$$f_t(x) = F_t e^{-\nu_t x},$$

(6.30)

i.e. a power-law correction in $\ell$. $\nu_{t(\alpha)}$ is a new universal critical exponent governing the corrections to the scaling of $\tilde{S}_\alpha$, analogous to the one introduced in clean systems (cf. Chapter 4). We can see that $\nu_{t(\alpha)}$ decreases with increasing $\alpha$, but a precise numerical estimate is difficult. And the accuracy of our results does not allow to establish numerically an exact formula for the $\alpha$ dependence of the exponent. We also mention that the corrections to the scaling are of the same form also in ab-initio calculations, as qualitatively clear from Fig. 6.6. This shows the correctness of the RSP description and also that the real spin-chain does not introduce new leading corrections to the scaling in addition to the RSP ones.

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Figure 6.7: Correction to the scaling - Scaling functions for the correction to the scaling $f_t(S)$ in Eq. (6.26) obtained as difference between $S_{\text{odd}}^{\alpha}(\ell)$ and $S_{\text{even}}^{\alpha}(\ell)$. Full and dashed lines correspond to uniform and exponential distributions of disorder respectively.

Figure 6.8: Dependence on the disorder distribution - $\tilde{S}_\alpha$ for two disorder distributions. The RSP data are for chains of 10000 spins and averaged over 320000 configurations.
6.3.4 Universality

All the results presented so far, both ab-initio and RSP have been obtained for random distributions of the coupling constant $J$ in the interval $[0, 1]$. However, the universal prediction of RSRG must be independent of the distributions of $J$ (as long as new symmetries are not introduced). We check this universality by studying the RSP chain with $L = 10000$ spins with coupling distributed both uniformly $J \in [0, 1]$ and exponentially $P(J) \sim e^{-J}$. In Fig. 6.8 we report the numerical RSP results of $\hat{S}_\alpha$ for $\alpha = 1, 2$ and two distributions of the disorder. As expected, the two distributions lead to slightly different results: only the leading logarithmic term in $\ell$ is universal, while the additive constant term is not.

![Figure 6.9: Universality of the scaling function](image)

Figure 6.9: Universality of the scaling function - $\hat{S}_\alpha$ as function of $S_\alpha$ for $\alpha = 2.9$ and for two disorder distributions (RSP data with $L = 10000$ and 320000 configurations). The scaling function is disorder independent.

To check the universality of the leading term, Fig. 6.9 reports $\hat{S}_\alpha$ against $S_\alpha$ for $\alpha = 2.9$ (other values of $\alpha$ lead to equivalent plots) for the two distributions. The two curves perfectly coincide, despite they are different when plotted as functions of $\ell$. This means that all the non-universal behavior of the additive constants is washed out and we are left with a universal function. At first this result can seem surprising, but it is easy to realize that, in this kind of plots, the dependence on the non-universal cut-off, or lattice spacing $a$, disappears and the leftover difference of non-universal additive constants is universal. For example, for the conformal entropies we have the universal relation

$$ S_{\alpha}^{CFT} = \frac{S_{\alpha}^{CFT}}{2} \left( 1 + \frac{1}{\alpha} \right) + c'_\alpha - \frac{c'_{\alpha}}{2} \left( 1 + \frac{1}{\alpha} \right) , $$

where evidently the $a$ dependence disappeared.
Having established that both $A_t$ and $B_t$ are universal, we reconsider our results for the disordered systems. We have already discussed for the uniform distribution (see Fig. 6.5) how the numerical value of $A_t$ agrees with the analytical RSRG prediction. The independence of $A_t$ on the disorder distribution confirms its universality. In Fig. 6.10 we plot the quantity

$$\Delta = \tilde{S}_0^{-\alpha} - \frac{g_\mu(t(\alpha))}{1 - \alpha},$$

where $g_\mu(t)$ is the function in Eq. (6.16) and $\mu$ is fixed by $S_\alpha$ via $\mu = \frac{3}{\ln 2}S_\alpha + \frac{1}{3}$. This quantity has been built in such a way to cancel the leading behavior $A_t$ so to leave only $B_t$. Albeit little noisy, Fig. 6.10 shows clearly the disorder independence of $B_t$.

**Figure 6.10: Universality of $B_t$.** The quantity $\Delta$ defined in Eq. (6.32) vs $S_\alpha$ for uniform and exponential distributions of disorder. With varying $\alpha$ the two differences are the same, showing the universality of the coefficient $B_t(\alpha)$.

Disappointingly, as shown for uniform disorder, the RSP and ab-initio calculation for $\tilde{S}_\alpha$ provide different values for the constant $B_t(\alpha)$ that are both different from the RSRG expression in Eq. (6.18). On the one hand, this is showing that the RSP description is unable to catch this feature of the spin-chain because numerical RSP and ab-initio data disagree. On the other hand, this is also showing that while carrying out the analytic results for $g(t)$, some of the assumptions made influence significantly this quantity. There are two possible explanations to motivate the last discrepancy. One is that the distribution $f(\mu)$ in Eq. (6.12) contains some additional (subleading) terms not considered here. In fact, as already discussed, Eq. (6.12) has been deduced neglecting terms coming from the starting disorder distribution and it is only asymptotically true. The other possibility is instead that the discarded terms in the renewal equation (6.13) contribute to $B_t$. Several pieces of information have been indeed ignored: memory beyond first order, multiple decimations, the flow of the distribution to the critical
point, etc. We believe it is rather improbable that \( f(\mu) \) should be modified. It is difficult to imagine how to modify it keeping all the other correct results (i.e. the entanglement entropy, \( A_t \), etc.). On the other hand, solving the renewal equation in the presence of the discarded effects is very hard (maybe impossible). Thus, to convince oneself that these processes can be responsible of a changing in \( B_t \), we try to add some oversimplified processes to the renewal equation. For example we could modify Eq. (6.15) as follows:

\[
 g(\mu)(t) = \ln \left[ \mathcal{Z}^{-1} \left\{ \frac{1}{s} \frac{G(\tilde{f}(s))}{G(e^{\gamma s})} \right\}^{\mu} \right],
\]

(6.33)

where \( G \) is a non-singular function such that \( G(1) = 0 \). In particular if \( G \) is linear we get Eq. (6.15). And the subsequent terms in the series expansion of \( G \) could be interpreted as an effective description of processes involving multiple decimations. Actually, all these processes change \( B_t \), but leave \( A_t \) unchanged, showing that this is the most probable explanation of the discrepancy. However, from the ab-initio results, we know that the real spin-chain introduces further corrections to this term and so we do not find reasonable to embark in a difficult calculation, that in any case will not provide the correct answer for the spin-chain.

To conclude the universality section, it is worth to mention that the oscillating corrections to the scaling (the function \( f_t \) in Eq. (6.26)) also do not depend on the disorder distribution as shown in Fig. 6.7 confirming their universality.

In this chapter we provided an analytical and numerical description of the R\'enyi entropies \( S_\alpha \) and \( \tilde{S}_\alpha \) in a random singlet phase. For \( S_\alpha \) the leading logarithmic behavior is \( \alpha \)-independent and only the subleading non-universal constant term depends on \( \alpha \). Oppositely, the leading universal term of \( \tilde{S}_\alpha \) has a non-trivial \( \alpha \)-dependence. The functions \( A_t \) and \( B_t \) connecting linearly \( \tilde{S}_\alpha \) and \( S_\alpha \) are both independent of the cut-off length introduced by the chain, and so universal. We determined analytically the coefficient \( A_t \) by solving the real-space renormalization group equations, however the approximations done in the RG equations do not allow the determination of the subleading universal constant. We also studied the finite-size scaling: for finite chains the above relations still hold if the subsystem length \( \ell \) is replaced by a modified chord length that is phenomenologically well approximated by Eq. (6.25). However there is no theoretical explanation for this finite-size scaling form.
Recent experiments on trapped cold atomic gases \cite{Kinoshita1, Kinoshita2, Kinoshita3} have raised intriguing fundamental questions regarding the non-equilibrium dynamics of correlated many-body quantum systems. These cold atom systems are sufficiently weakly coupled to their environments as to allow the observation of essentially unitary nonequilibrium time evolution on long time scales. The quantum Newton’s cradle experiments of Kinoshita et al \cite{Kinoshita1} in particular have focused the attention on the roles played by dimensionality and conservation laws.

The observed absence of “thermalization” in quasi one dimensional condensates was attributed to the experimental system being approximately describable by a quantum integrable many-body theory. This in turn initiated vigorous research on clarifying the role played by quantum integrability in determining the stationary (late time) behaviour of nonequilibrium evolution in correlated quantum systems \cite{Integrability1, Integrability2, Integrability3, Integrability4, Integrability5, Integrability6, Integrability7, Integrability8, Integrability9, Integrability10, Integrability11, Integrability12, Integrability13, Integrability14, Integrability15, Integrability16}. The simplest way of driving a quantum system out of equilibrium is by means of a quantum quench: a system is prepared in the ground state of a given Hamiltonian $H(h_0)$, where $h_0$ is an experimentally tuneable parameter such as a bulk magnetic field. At time $t = 0$ the parameter $h_0$ is changed suddenly to a different value $h$ and one then considers the unitary time evolution of the system by means of the new Hamiltonian $H(h)$

$$\Psi(t) = e^{-iH(t)\hat{t}} \Psi_0, \quad H(h_0) \Psi_0 = E_0 \Psi_0$$  \hfill (7.1)

Central issues that have been investigated are whether the system “relaxes” to a stationary state, and if it does, how to characterize its physical properties at late times. Relaxation of a state evolving unitarily can appear strange. The correct query should be whether every “accessible” observable relaxes. In fact, in an infinite system only local operators can be associated to observables: we do not have access to the entire system. This means that we can not “see” that the state is pure, and the lack of information about non-local operators can be taken into account by tracing out the inaccessible degrees of freedom, considering the reduced density matrix associated to the accessible part $A$ of the system

$$\rho_A(t) \equiv \text{Tr}_A(\Psi(t)\langle \Psi(t) \rangle)$$ \hfill (7.2)

This is completely equivalent to work with the density matrix of the entire system but considering only the expectation values of local operators. However, this different point of view has
7. QUANTUM QUENCHES

the advantage of encoding the issue of locality in a single operator $\rho_A$. If the limit $t \to \infty$ exists for arbitrary large subsystem’s size $\ell = |A|$, the physical properties at late times are described by the density matrix

$$\bar{\rho}_A = \lim_{t \to \infty} \rho_A(t). \quad (7.3)$$

It is widely believed (see e.g. [117] for a comprehensive summary) that the behaviour of local observables can be described in terms of either an effective thermal (Gibbs) distribution

$$\bar{\rho}_A \xrightarrow{\ell \gg 1} e^{-\beta H_A} \frac{Z}{Z}, \quad (7.4)$$

where $H_A$ is the Hamiltonian restricted to the subspace $A$, or a generalized Gibbs ensemble (GGE) [19][103], which we are going to describe in the next section. It has been argued that the latter arises for integrable models, while the former obtains for generic systems. However, several recent studies [113][114][115][116] suggest that the behaviour is more complicated and in particular depends on the initial state. Moreover, open questions remain even with regards to the very existence of stationary states. Indeed oscillations can survive the large time limit and, in general, we could expect

$$\rho_A(\ell) \xrightarrow{\ell \gg \ell \gg 1} \bar{\rho}_A + \sum_n \left[ e^{i\omega_n t} \rho_n + h.c. \right]. \quad (7.5)$$

For example the order parameter of certain mean-field models have recently been shown to display persistent oscillations [118][119][120][121][122][123][124].

Finally, we stress we are considering the time evolution of a state that, at the initial time, is the ground state of a local Hamiltonian. It is not the most general state, as it should be evident, by now. In particular correlation functions blow over with the distance. The final Hamiltonian is local too. This features open the way for a semi-classical interpretation [125]. In fact several aspects of the time-evolution have been explained by the picture of ballistically moving quasi-particles spontaneously created after the quench [15], as we are going to show in the following sections.

7.1 Thermalization vs. GGE

Here we consider the issue of thermalization in 1D systems. We start with non-integrable models. In Chapter 2 we introduced the concept of integrability and we claimed that, in spin chains, it can be related to the existence of an infinite set of local conservation laws [56]. This automatically defines the opposite concept of non-integrable system which, however, includes a wide variety of models with different features. We confine ourself to the models in which there is no local operator commuting with the Hamiltonian, except for the energy density itself. If the large-time limit $t \to \infty$ exists the reduced density matrix $\bar{\rho}_A$ must be written in terms of
$H_A$ as a matter of course: any other operator in $A$ would have a non-trivial dependence on time. If we would be pedantic, the stationary condition should be written as

$$\lim_{t \to \infty} \text{Tr}_\bar{A} \left[ [H, \rho(t)] \right] = 0$$

(7.6)

i.e.

$$[H_A, \bar{\rho}_A] = \lim_{t \to \infty} \sum_{ij} \sqrt{p_i} p_j \left[ e^{i(\omega_i(t) - \omega_j(t))} \langle \phi_i | \rho(t) \langle \phi_j | e^{i(\bar{\omega}_i(t) - \bar{\omega}_j(t))} | \bar{\phi}_i \rangle \langle \bar{\phi}_j | V | \bar{\phi}_i \rangle \right],$$

(7.7)

where $p_i$ and $e^{i\omega_i(t)} | \phi \rangle$ are the eigenvalues and the eigenvectors of $\rho_A(t)$, respectively, while $e^{i\bar{\omega}_i(t)} | \bar{\phi} \rangle$ are the corresponding eigenvectors of $\bar{\rho}_A(t)$, obtained applying the Schmidt decomposition to $\rho(t)$. The operator $V$ is the interaction between $A$ and $\bar{A}$, that is to say $H = H_A + H_{\bar{A}} + V$.

In order to isolate the time dependence in Eq. (7.7) we used that at late time both $\rho_A(t)$ and $\bar{\rho}_A(t)$ become independent of time, hence the time dependence must be simply in the phase of eigenvectors (assuming non-degeneracy, as we would expect in non-integrable models). Prompted by the lack of symmetries, we guess that only the diagonal terms in the r.h.s. of Eq. (7.7) could be different from 0. However $\text{Tr}_\bar{A} V$, which eventually would appear in the r.h.s. of Eq. (7.7), is 0 because $V$ acts non-trivially both on $A$ and on $\bar{A}$, that is to say it cannot include a term proportional to the identity (the only operator with trace different from 0) in the space $\bar{A}$. Thus, we find the natural result expected from the beginning

$$[H_A, \bar{\rho}_A] \xrightarrow{t \to \infty} 0.$$  

(7.8)

As a consequence, $\bar{\rho}_A = \bar{\rho}_A[H_A]$. However, if there are some symmetries, e.g. a finite rotational invariance, the time dependence in Eq. (7.7) could be more complicated and the non-diagonal matrix elements of $V$ do contribute to the late time behavior. Actually $V$ is local and it is natural to expect that the r.h.s. of Eq. (7.7) would result just in a corrective boundary term.

In statistical mechanics, the functional dependence of the density matrix on the Hamiltonian follows from the principle of maximum entropy. It is believed that the analogous principle of maximum entanglement entropy still applies in our context. Because the energy density is conserved, the maximization of the entanglement entropy gives the thermal-like distribution

$$\bar{\rho}_A \sim \frac{e^{-\beta H_A}}{Z},$$

(7.9)

where $\beta$ is found by imposing the energy conservation. The importance of locality can be understood by observing that the thermal distribution relies on the assumption of approximate separability

$$\frac{\log \bar{\rho}_{A_1 \cup A_2}}{\ell_1 + \ell_2} \approx \frac{\log \bar{\rho}_{A_1} \oplus \log \bar{\rho}_{A_2}}{\ell_1 + \ell_2} + o(\ell_1^0, \ell_2^0),$$

(7.10)

which is strongly related to the locality of the interaction in $\log \rho$ (otherwise we could have substituted $H_A$ with any function of $H_A$, e.g. the operator $H_A^2$). Eq. (7.10) is a non-trivial statement that can not be verified easily: $A_1 \cup A_2$ is in a mixed state, hence we can not even use the entanglement entropies to measure the entanglement between $A_1$ and $A_2$. Actually, there is
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no proof of the approximate separability, as well as of the principle of maximum entanglement entropy. And in the following, we will assume them, without any further justification. The analysis of quench dynamics in several models has been confirming this picture, up to now. However there are numerical indications that non-thermal distributions could arise [116].

If, besides the Hamiltonian, there are other conserved local quantities $I_k$, the maximization of entanglement entropy gives

$$\bar{\rho}_A \sim \frac{e^{-\beta H_A + \sum_n \mu_n f^{(n)}_A}}{Z}, \quad (7.11)$$

where the sum is over all local independent operators (almost) commuting with the Hamiltonian (restricted to the space $A$). The Lagrange multipliers $\mu_n$ are found by imposing the conservation laws. When the system is integrable there are infinite local conserved quantities and the distribution (7.11) is the so-called GGE (generalized Gibbs ensemble). We point out that if we consider the evolution by means of the Hamiltonian

$$\bar{H} = H - \frac{1}{\beta} \sum_n \mu_n f^{(n)}_A, \quad (7.12)$$

we expect the subsystem to relax to the same stationary state as before. Indeed the parameters $\beta$ and $\mu_n$ are completely determined by the initial state: because $[H, \bar{H}] = 0$ the final state can not be different. However, in this way we are assuming implicitly also the existence of an asymptotic stationary state when the evolution is driven by $\bar{H}$. In order to make things a little clearer we could consider, after a large time $t$ in which the evolution is driven by $H$, a further evolution for a time $\bar{t} \gg t$ with the Hamiltonian $\bar{H}$. Because the state is already in an almost thermal state of $\bar{H}$ we surmise nothing more happens, besides the fact that the final state would be even better approximated by a thermal state. If we now consider the evolution with $-H$, for a time $t$ equal to the initial one, we recover simply the evolution with $\bar{H}$

$$e^{iHt} e^{-i\bar{H}t} e^{-iHt} = e^{-i\bar{H}t}. \quad (7.13)$$

Because $t \ll \bar{t}$ we expect the further evolution to be be unable to move the system from the state, which is very close to a thermal one (we remind $[H, \bar{H}] = 0$). This means that, eventually, the state has thermalized at inverse temperature $\beta^{-1}$. The memory of the initial state is retained by $\bar{H}$.

In the picture presented so far we never worried about correlation lengths, and the GGE is expected to be an effective description of the state at late times after a global quench both for critical and non-critical systems. In the subsection below we consider the case when $H$ is the Hamiltonian of a CFT. We observe without further ado that this is not completely equivalent to consider an Hamiltonian $\bar{H}$ whose underlying limit is a CFT, because the entire spectrum of the Hamiltonian plays a role in the evolution after a (global) quench.
7.1 Thermalization vs. GGE

7.1.1 CFT

The evolution of the entanglement entropy of a subsystem in the limit of large length after a global quench in a 1+1 dimensional CFT has been obtained in Ref. [15]. The evolution of correlation functions has been investigated in Refs. [16] and [126]. Here we review the main results, which constitute the starting point for any interpretation of quench dynamics.

Let us consider a 1D lattice quantum theory. The lattice spacing is $a$, and the lattice variables are labelled by a discrete variable $x$. Time is considered to be continuous. The dynamics of the theory is described by the hamiltonian $H$. The system is prepared in a state $|\psi_0\rangle$ that is not an eigenstate of $H$. At time $t = 0$ the unitary evolution with $H$ ensues. The expectation value of a local operator $O(\{x_i\})$ at time $t$ is

$$\langle O(t, \{x_i\}) \rangle = \langle \psi_0 | e^{iHt} O(\{x_i\}) e^{-iHt} | \psi_0 \rangle.$$  

(7.14)

In order to make the path integral representation absolutely convergent, we include damping factors $e^{-\epsilon H}$ into the time-dependent expectation value as follows:

$$\langle O(t, \{x_i\}) \rangle = Z^{-1} \langle \psi_0 | e^{iHt-\epsilon H} O(\{x_i\}) e^{-iHt-\epsilon H} | \psi_0 \rangle.$$  

(7.15)

The normalization factor $Z = \langle \psi_0 | e^{-2\epsilon H} | \psi_0 \rangle$ ensures that the expectation value of the identity is one. At the end of the calculation we shall set $\epsilon$ to zero.

Eq. (7.15) may be represented by an analytically continued path integral in imaginary time over the field variables $\phi(\tau, x)$, with initial and final values weighted by the matrix elements with $|\psi_0\rangle$:

$$\int [d\phi(\tau, x)] \langle \psi_0 \phi(\tau_2, x) \rangle \langle \phi(\tau_1, x) | \psi_0 \rangle e^{-\int_{\tau_1}^{\tau_2} L(\phi)d\tau}$$  

(7.16)

where $\int_{\tau_1}^{\tau_2} L(\phi)d\tau$ is the (euclidean) action. The operator $O$ is inserted at $\tau = 0$, and the width of the slab is $2\epsilon$. Eventually, $\tau_1$ and $\tau_2$ should be continued to their effective values $\pm \epsilon - i\tau$. We are assuming that the leading asymptotic behavior given by field theory, which applies to the Euclidean region (large imaginary times), may simply be analytically continued to find the behavior at large real time.

Our system is at a (quantum) phase transition. Thus, for the purpose of extracting the asymptotic behavior, as long as $|\psi_0\rangle$ is translationally invariant, we may replace it by the appropriate RG-invariant boundary state $|\psi_0^*\rangle$ to which it flows. The difference may be taken into account, to leading order, by assuming that the RG-invariant boundary conditions are not imposed at $\tau = \tau_1$ and $\tau_2$ but at $\tau = \tau_1 - \tau_0$ and $\tau = \tau_2 + \tau_0$, being $\tau_0$ the so-called extrapolation length [127]. It characterizes the RG distance of the actual boundary state from the RG-invariant one. The effect of introducing $\tau_0$ is simply to replace $\epsilon$ by $\epsilon + \tau_0$. The limit $\epsilon \to 0^+$ can now safely be taken, so the width of the slab is then taken to be $2\tau_0$. In the following we will consider the equivalent slab geometry between $\tau = 0$ and $\tau = 2\tau_0$ with the operator $O$ inserted at $\tau = \tau_0 + i\tau$. 

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In our case, RG-invariant boundary conditions correspond to conformally invariant boundary states. The slab geometry of above is just a two-dimensional strip whose points are labelled by a complex number \( w = x + i \tau \) with \( 0 < \text{Im} w < 2 \tau_0 \). The strip can be obtained from the upper half-plane \( \text{Im} z > 0 \) by the conformal mapping

\[
w(z) = \frac{2 \tau_0}{\pi} \log z,
\]

with the images of points at the same imaginary time on the strip lying along \( \text{arg} z = \theta = \pi \tau / (2 \tau_0) \). In the case where \( \mathcal{O} \) is a product of local primary scalar operators \( \Phi_i(w_i) \), the expectation value in the strip is related to the one in the upper half-plane (UHP) by the standard transformation

\[
\langle \prod_i \Phi_i(w_i) \rangle_{\text{strip}} = \prod_i |w_i'(z_i)|^{-y_i} \langle \prod_i \Phi_i(z_i) \rangle_{\text{UHP}},
\]

where \( y_i \) is the bulk scaling dimension of \( \Phi_i \). The expectation values of the \( \Phi_i \)'s in the ground state of \( H \) are supposed to have been subtracted off. The asymptotic real time dependence is obtained via the analytic continuation \( \tau \to \tau_0 + it \), and taking the limit \( t, r_{ij} \gg \tau_0 \).

The one-point function. In the UHP, the one-point function of a scalar primary field with bulk scaling dimension \( y \) is \( \langle \Phi(z) \rangle_{\text{UHP}} = A^\Phi_b [2 \text{Im}(z)]^{-y} \). The normalization factor \( A^\Phi_b \) is a non-universal amplitude. In CFT the normalizations are chosen in such a way that the bulk two-point functions have unit amplitude (i.e. \( \langle \Phi(z_1) \Phi(z_2) \rangle_{\text{bulk}} = |z_2 - z_1|^{-2y} \)). This choice fixes unambiguously the amplitude \( A^\Phi_b \) that turns out to depend both on the considered field \( \Phi \) and on the boundary condition on the real axis \( b \). It vanishes if \( \Phi \) corresponds to an operator whose expectation value in \( |\psi_0 \rangle \) vanishes, and thus \( \langle \Phi(t) \rangle = 0 \), for all times.

When the primary field is not vanishing on the boundary, performing the conformal mapping \ref{eq:7.17} we obtain

\[
\langle \Phi(w) \rangle_{\text{strip}} = |w'(z)|^{-y} \langle \Phi(z(w)) \rangle_{\text{UHP}} = A^\Phi_b \left[ \frac{\pi}{4 \tau_0 \sin(\pi \tau / (2 \tau_0))} \right]^y
\]

that continued to real time \( \tau = \tau_0 + it \) gives

\[
\langle \Phi(t) \rangle = A^\Phi_b \left[ \frac{\pi}{4 \tau_0 \cosh(\pi t / (2 \tau_0))} \right]^y \approx A^\Phi_b \left( \frac{\pi}{2 \tau_0} \right)^y e^{-y \pi t / 2 \tau_0}.
\]

Thus the order parameter (and any other observable described by a primary field) decays exponentially in time to the ground-state value, with a non-universal relaxation time \( t^\text{rel}_0 = 2 \tau_0 / y_0 \pi \).

The ratio of the relaxation times of two different observables equals the inverse of the ratio of their scaling dimensions and it is then universal.

The two-point function. The two-point function in the half-plane has the general form

\[
\langle \Phi(z_1) \Phi(z_2) \rangle_{\text{UHP}} = \left( \frac{z_{12} z_{21}}{z_{12} z_{12} z_{11} z_{22}} \right)^y F(\eta) \quad \eta = \frac{z_{21} z_{22}}{z_{12} z_{21}},
\]

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where $\eta$ is the four-point ratio and the function $F(\eta)$ depends explicitly on the considered model. $z_{ij} = |z_i - z_j|$ and $\bar{z}_i$. Under the conformal map to the strip the first part of Eq. (7.21) transforms as follows

$$
\left(\frac{z_{12}z_{21}}{z_{12}z_{21}z_{11}z_{22}}\right)^y \rightarrow \left(\frac{\pi}{2\tau_0}\right)^2 \frac{\cosh(\pi x/2\tau_0) - \cos(\pi \tau/\tau_0)}{8 \sinh^2(\pi x/4\tau_0) \sin^2(\pi \tau/2\tau_0)} \right)^y, \tag{7.22}
$$

that continued to real time $\tau = \tau_0 + it$ gives

$$
\langle \Phi(x,t)\Phi(0,t) \rangle = \left(\frac{\pi}{2\tau_0}\right)^2 \frac{\cosh(\pi x/2\tau_0) + \cosh(\pi t/\tau_0)}{8 \sinh^2(\pi x/4\tau_0) \cosh^2(\pi t/2\tau_0)} \right)^y |F(\eta)|_{\text{strip}}. \tag{7.23}
$$

Thus we need only to map $F(\eta)$ that, in the general case, is an unknown function. Actually, in order to get the asymptotic behavior of the two-point function we only need to know the behavior close to $\eta \sim 0$ (i.e. the behavior close to the surface) and for $\eta \sim 1$ (i.e. deep in the bulk). They are both exactly known. Indeed when $\eta \sim 1$ the two points are deep in the bulk, meaning $F(1) = 1$. Instead for $\eta \ll 1$, from the short-distance expansion, we have

$$
F(\eta) \simeq (A^b_h)^2 \eta^{y_b}, \tag{7.24}
$$

where $y_b$ is the boundary scaling dimension of the leading boundary operator to which $\Phi$ couples and $A^b_h$ is the same coefficient as in Eq. (7.20) [see e.g. Ref. [129]].

Finally we get

$$
\left\{ \begin{array}{ll}
\langle \Phi(r,t)\Phi(0,t) \rangle \propto (A^b_h)^2 e^{-x \pi t/\tau_0} \propto e^{\pi y_b (t-r)/\tau_0} & t < r/2 \\
\langle \Phi(r,t)\Phi(0,t) \rangle \propto e^{-x \pi r/2\tau_0} & t > r/2.
\end{array} \right. \tag{7.25}
$$

If $\langle \Phi \rangle \neq 0$, $y_b = 0$ and the last factor is absent. The leading term is then just $\langle \Phi \rangle^2$. Thus the leading term in the connected two-point function vanishes for $t < r/2$, and its first non-vanishing contributions are given by subleading terms either in $F$ or in the bulk-boundary short-distance expansion.

Moreover, the behavior within a distance $\sim \tau_0$ of the horizon $r = 2t$ depends on the detailed form of $F$.

**Entanglement entropies.** In section 1.2.1 we have computed the entanglement entropies of spin blocks in conformal systems. The asymptotic expression for the evolution of the entanglement entropies after a global quench can be obtained by following the same procedure. In brief, the moments of the reduced density matrix associated to the block $A$ can be written as the correlation function of local operators $\Phi_{\pm n}$ located at the branch points (twist fields), which transforms simply under conformal mappings. By taking the image of the branch points to be $z_1 = e^{-\pi t/4\tau_0} e^{i \pi r/2\tau_0}$ and $z_2 = e^{\pi t/4\tau_0} e^{i \pi r/2\tau_0}$ [15], from [3] in the $z$-plane we have

$$
\text{Tr} \rho_A^n = \langle \Phi_A \Phi_{-n} \rangle \sim c_n \left(\frac{|z_1 - z_2||z_2 - \bar{z}_1|}{|z_1 - z_2||\bar{z}_2 - \bar{z}_1||z_1 - \bar{z}_1||z_2 - \bar{z}_2|}\right)^{h_n} \tilde{F}_n(\eta), \tag{7.26}
$$

where $z_{ij} = |z_i - z_j|$ and $\bar{z}_i$. Under the conformal map to the strip the first part of Eq. (7.21) transforms as follows

$$
\left(\frac{z_{12}z_{21}}{z_{12}z_{21}z_{11}z_{22}}\right)^y \rightarrow \left(\frac{\pi}{2\tau_0}\right)^2 \frac{\cosh(\pi x/2\tau_0) - \cos(\pi \tau/\tau_0)}{8 \sinh^2(\pi x/4\tau_0) \sin^2(\pi \tau/2\tau_0)} \right)^y, \tag{7.22}
$$

that continued to real time $\tau = \tau_0 + it$ gives

$$
\langle \Phi(x,t)\Phi(0,t) \rangle = \left(\frac{\pi}{2\tau_0}\right)^2 \frac{\cosh(\pi x/2\tau_0) + \cosh(\pi t/\tau_0)}{8 \sinh^2(\pi x/4\tau_0) \cosh^2(\pi t/2\tau_0)} \right)^y |F(\eta)|_{\text{strip}}. \tag{7.23}
$$

Thus we need only to map $F(\eta)$ that, in the general case, is an unknown function. Actually, in order to get the asymptotic behavior of the two-point function we only need to know the behavior close to $\eta \sim 0$ (i.e. the behavior close to the surface) and for $\eta \sim 1$ (i.e. deep in the bulk). They are both exactly known. Indeed when $\eta \sim 1$ the two points are deep in the bulk, meaning $F(1) = 1$. Instead for $\eta \ll 1$, from the short-distance expansion, we have

$$
F(\eta) \simeq (A^b_h)^2 \eta^{y_b}, \tag{7.24}
$$

where $y_b$ is the boundary scaling dimension of the leading boundary operator to which $\Phi$ couples and $A^b_h$ is the same coefficient as in Eq. (7.20) [see e.g. Ref. [129]].

Finally we get

$$
\left\{ \begin{array}{ll}
\langle \Phi(r,t)\Phi(0,t) \rangle \propto (A^b_h)^2 e^{-x \pi t/\tau_0} \propto e^{\pi y_b (t-r)/\tau_0} & t < r/2 \\
\langle \Phi(r,t)\Phi(0,t) \rangle \propto e^{-x \pi r/2\tau_0} & t > r/2.
\end{array} \right. \tag{7.25}
$$

If $\langle \Phi \rangle \neq 0$, $y_b = 0$ and the last factor is absent. The leading term is then just $\langle \Phi \rangle^2$. Thus the leading term in the connected two-point function vanishes for $t < r/2$, and its first non-vanishing contributions are given by subleading terms either in $F$ or in the bulk-boundary short-distance expansion.

Moreover, the behavior within a distance $\sim \tau_0$ of the horizon $r = 2t$ depends on the detailed form of $F$.
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where \( h_n = (c/12)(n - 1) \). Actually, the function \( \tilde{F}_n(\eta) \) is irrelevant. Indeed, after the conformal mapping (7.17) and in the limit of large \( \ell \) and \( t \), the four-point ratio \( \eta \) is mapped to \( \theta(2t - \ell) \), so that we only need the behavior of \( \tilde{F}_n \) close to \( \eta \approx 0 \) and \( \eta \approx 1 \). However, even if \( \tilde{F}_n \) is generally unknown, \( \tilde{F}_n(1) = \tilde{F}_n(0) = 1 \) [34]. Under the conformal mapping (7.17)

\[
\langle \Phi_n(w_1)\Phi_{-n}(w_2) \rangle = |w'(z_1)w'(z_2)|^{-h_n} \langle \Phi_n(z_1)\Phi_{-n}(z_2) \rangle
\]

(7.27)

and continuing to \( \tau = \tau_0 + it \), we eventually find [15]

\[
\text{Tr} \rho^a_n(t) \sim c_n(\pi/2\tau_0)^{2h_n} \left( \frac{e^{\pi \ell/2\tau_0} + e^{-\pi \ell/2\tau_0} + 2 \cosh(\pi t/\tau_0)}{(e^{\pi \ell/4\tau_0} - e^{-\pi \ell/4\tau_0})^2 \cosh^2(\pi t/2\tau_0)} \right)^{h_n}.
\]

(7.28)

In the case where \( \ell/\tau_0 \) and \( t/\tau_0 \) are large this simplifies to

\[
c_n(\pi/2\tau_0)^{2h_n} \left( \frac{e^{\pi \ell/2\tau_0} + e^{\pi t/\tau_0}}{e^{\pi \ell/2\tau_0} - e^{\pi t/\tau_0}} \right)^{h_n}.
\]

(7.29)

Finally, by differentiating with respect to \( n \) we get the entropy (replica trick),

\[
S_A(t) \sim -\frac{c}{3} \log \tau_0 + \left\{ \begin{array}{ll}
\frac{\pi c t}{6\tau_0} & t < \ell/2 \\
\frac{\pi c \ell}{12\tau_0} & t > \ell/2
\end{array} \right.
\]

(7.30)

\( S_A(t) \) increases linearly until it saturates at \( t = \ell/2 \). The sharp cusp in this asymptotic result is rounded over a region \( |t - \ell/2| \sim \tau_0 \).

Notice that both correlation functions and entanglement entropies at late times after a quench in CFT have the same behavior as in the thermal state at inverse finite temperature \( \beta_{\text{eff}} = 4\tau_0 \): any finite subsystem \( A \) reaches a quasi-stationary thermal state, in which the infinite remaining part of the system acts as a thermal bath. In fact, it has been shown that, within CFT, this effective temperature is the same for any observable [126] and so can be properly defined. This is due essentially to the fact that the dispersion relation in CFT is exactly linear, i.e. a single velocity comes into play. In the following sections we consider quenches in the XY model. First we consider the time evolution of entanglement and then we study the order parameter in the Ising model.

7.2 “Non-interacting” chains

Quench dynamics finds a natural framework in the models that can be mapped into free fermions (see Chapter 2). In fact, if both \( H_0 \) and \( H \) are quadratic in the Majorana fermions Eq. (2.35), because the time-evolution operator \( e^{-itH} \) is the exponential of a quadratic form, from Eqs. (3.19) it follows that Wick theorem applies at any time \( t \) and the correlation matrix \( \Gamma \) is given by

\[
\Gamma(t) = e^{-\mathcal{H}t} \Gamma_0 e^{\mathcal{H}t} \quad \text{with} \quad H = \frac{1}{4} \sum_{l,n} a^*_l \mathcal{H}_{ln} a_n.
\]

(7.31)

Considering quenches in the XY model, the matrices \( \mathcal{H} \) and \( \Gamma_0 \) are block diagonalized by the same transformation, indeed the Jordan-Wigner transformation and the Fourier transform do
7.2 “Non-interacting” chains

not depend on the particular system and the remaining Bogolioubov transformation mixes only two modes (cf. Sec. 2.1.1). The effective dynamics is two-dimensional and the correlation matrix can be written in closed form at any time after the quench. In particular we find

$$\Gamma(t)_{ln} = \frac{1}{L} \sum_{k=1}^{L} e^{-i(n-l)\varphi_k} e^{-i\frac{\Delta_k}{2} \sigma_z} e^{-i\xi \sigma_y} e^{i\frac{\Delta_k}{2} \sigma_z} e^{-i\frac{\Delta_k}{2} \sigma_y}$$, 

(7.32)

where $\theta_k$ and $\varepsilon_k$ are the Bogolioubov angle and the dispersion relation of the final Hamiltonian, respectively. $\Delta_k \equiv \theta_k - \theta_k^0$ is the difference between the Bogolioubov angles of the two Hamiltonians. In the thermodynamic limit the sum must be turned into an integral and we get

$$\Gamma(t)_{ln} = \int_0^{2\pi} \frac{d\varphi}{2\pi} e^{-i(n-l)\varphi} e^{-i\frac{\Delta}{2} \sigma_z} e^{-i\xi \sigma_y} e^{i\frac{\Delta}{2} \sigma_z}.$$ 

(7.33)

As long as we are interested in the expectation value of local operators, the limit of large times can be taken directly in the correlation matrix itself, obtaining

$$\Gamma^{(\infty)}_{ln} \equiv \lim_{t \to \infty} \Gamma(t)_{ln} = \int_0^{2\pi} \frac{d\varphi}{2\pi} e^{-i(n-l)\varphi} \cos \Delta \ e^{-i\frac{\Delta}{2} \sigma_z} \ e^{i\frac{\Delta}{2} \sigma_z}.$$ 

(7.34)

Notice the the limit exists: late time after a quench in the XY model the state does relax. By comparing Eqs. (7.32), (7.33) and (7.34) we get a finite version of the correlation matrix at late times

$$[\Gamma^{(\infty)}_{(L)}]_{ln} = \frac{1}{L} \sum_{k=1}^{L} e^{-i(n-l)\varphi_k} \cos \Delta_k \ e^{-i\frac{\Delta_k}{2} \sigma_z} \ e^{i\frac{\Delta_k}{2} \sigma_z},$$

(7.35)

which indeed commutes with $H$, entering the quench parameter $\Delta$ just as a multiplicative factor (the matrix is block circulant). The correlation matrix $\bar{\Gamma}$ corresponding to the ground state of the Hamiltonian $\bar{H}$ is given by

$$\bar{\Gamma} = \text{sgn}[\Gamma^{(\infty)}] = \int_0^{2\pi} \frac{d\varphi}{2\pi} e^{-i(n-l)\varphi} \text{sgn}(\cos \Delta) \ e^{-i\frac{\Delta}{2} \sigma_z} \ e^{i\frac{\Delta}{2} \sigma_z}.$$ 

(7.36)

Notice that this correlation matrix corresponds to the excited state of $\bar{H}$ with characteristic function $m(\varphi) = -\text{sgn}(\cos \Delta)$ (see Chapter 5). This is an indirect check of the locality of the density energy: $|m(\varphi)| = 1$ (cos $\Delta$ is a smooth function of $\varphi$) means that the entanglement entropy of any connected subsystem grows as the logarithm of the subsystem’s length at the most, as expected for an Hamiltonian with local interaction. Actually something unexpected has happened. The quench parameter $|\cos \Delta|$ is equal to 1 for $\varphi = 0, \pi$, and other particular momenta depending on the quench. If we insist on determining $\bar{H}$ from Eq. (7.34) we find

$$H_{ln} \propto -\int_0^{2\pi} \frac{d\varphi}{2\pi} e^{-i(n-l)\varphi} \text{arctanh}(\cos \Delta) \ e^{-i\frac{\Delta}{2} \sigma_z} \ e^{i\frac{\Delta}{2} \sigma_z}.$$ 

(7.37)

so that its dispersion relation, i.e. $\varepsilon = -\text{arctanh}(\cos \Delta)$, shows some logarithmic singularities. By exploiting Eq. (5.20) we can see how these divergences modify the interaction

$$g_l \sim -\int_0^{2\pi} \frac{d\varphi}{2\pi} \text{arctanh}(\cos \Delta) e^{i\varphi} e^{-i\varphi}.$$ 

(7.38)
If $\cos \Delta$ were different from ±1 for any momentum, the interaction decays faster than any power. However, because of the logarithmic cut, it falls off like $1/r$. In fact, $\cos \Delta(\phi_k) = \pm 1$ means that $b_k^\dagger b_k$ commutes both with $H$ and with $H_0$, and we believe that this slow-decaying interaction is indeed due to the existence of conservation laws common to both Hamiltonians. We stress also that starting from a thermal state at finite temperature $\beta_0$, the state at late times is modified simply by a factor $\tanh(\beta_0 \epsilon(0)/2)$, multiplying $\cos \Delta$, so that singularities disappear ($|\tanh(\beta_0 \epsilon(0)/2)| < 1$) and the interaction falls off faster than any power.

In conclusion, the power law behavior of the interaction in the entanglement Hamiltonian $\tilde{H}$ late times after a quench in the XY model can be traced back to the fact that $H_0$ and $H$ have common conservation laws; however the slow-decaying behavior is canceled out by arbitrarily small thermal fluctuations at the initial time.

We have been able to draw this picture just analyzing the correlation matrix because the XY model is non-interacting. In general, in order to study the late time behavior, one has to follow the complete time evolution of observables, for many observables, as well as of the entanglement entropies. The discussion above about the locality of interaction in the entanglement Hamiltonian in our over simplified examples of quantum quenches gives an inkling of how things could be even more complicated. Indeed, the larger the range of interaction is in the entanglement Hamiltonian and the lesser the assumption of approximate separability (cf. Eq. (7.10)) is justified. And unusual dependences on the local conserved quantities could be in principle observed.

In the following subsection we report the results that we obtained in Ref. [12] for the evolution of entanglement entropies in the XY model after a quench.

### 7.2.1 Entanglement entropy

In Ref. [12] we provided the first (unique, up to now) analytic expression of the entanglement entropy at any time in the limit of a large block for the XY chain in a transverse magnetic field. We consider the quench with parameters suddenly changed at time $t = 0$ from $h_0, \gamma_0$ to $h, \gamma$.

Our main result is that, in the thermodynamic limit $L \to \infty$ and subsequently in the limit of a large block $\ell \gg 1$, the time dependence of $S_\ell(t)$ can be written as an integral over the momentum variable $\varphi$:

$$S_\ell(t) = t \int_{2|\epsilon'| \ell < \ell} \frac{d\varphi}{2\pi} 2|\epsilon'| H(\cos \Delta_\varphi) + \ell \int_{2|\epsilon'| \ell > \ell} \frac{d\varphi}{2\pi} H(\cos \Delta_\varphi),$$

(7.39)

where $\epsilon' = d\epsilon/d\varphi$ is the derivative of the dispersion relation $\epsilon^2 = (h - \cos \varphi)^2 + \gamma^2 \sin^2 \varphi$ and represents the momentum dependent sound velocity (that because of locality has a maximum we indicate as $v_M = \max_\varphi |\epsilon'|$), $\cos \Delta_\varphi = (hh_0 - \cos \varphi(h + h_0) + \cos^2 \varphi + \gamma \gamma_0 \sin^2 \varphi)/\epsilon_0$ contains all the quench information and $H(x) = e_1(1, x)$, defined in Eq. (2.131):

$$H(x) = -\frac{1 + x}{2} \log \frac{1 + x}{2} - \frac{1 - x}{2} \log \frac{1 - x}{2}.$$

(7.40)

In Ref. [15] an interpretation of the time dependence of $S_\ell$ has been provided in terms of causality (later generalized to the correlation functions in [16]). The idea is simple: the initial
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state has a very high energy relative to the ground state of the Hamiltonian which governs the
time evolution, and therefore acts as a source of quasiparticle excitations. Particles emitted from
different points (further apart than the correlation length in the initial state) are incoherent,
but pairs of particles moving to the left or right from a given point are entangled. Thus $S(t)$
should just be proportional to the number of coherent particles that emitted from any point
reach one a point in $[0, \ell]$ and the other the remainder of the system. Since there is a maximum
speed for these excitations $v_M$, this implies the linear growth for $2v_M t < \ell$ and saturation for
very large times.

However, only in the conformal case when $\epsilon'$ does not depend on the momentum because of
the linear dispersion relation, this scenario makes quantitative predictions on the time evolution,
else the rate of production of particles $f(p',p'')$ is an unknown function of the Hamiltonian
parameters both before and after the quench. The comparison of Eq. (7.39) with the general
one (Eq. (4.2) in [15]) allows to identify $f(p',p'')$ with $\delta(p' - p'')H(\cos \Delta \phi')$. We can also

easily read from our result the value of the ratio

$$R \equiv \frac{(\partial S_A/\partial t)_{t<\tau}}{2v_M(\partial S_A/\partial t)_{t>\tau}} = \frac{\int_{-\pi}^{\pi} d\phi' \epsilon'(\cos \Delta \phi')}{v_M \int_{-\pi}^{\pi} d\phi H(\cos \Delta \phi')} ,$$

(7.41)

that results to be the average of the absolute value of speed of the sound on the $H(\cos \Delta \phi)$
distribution. $R$ as function of the quench parameters is shown in Fig. [7.1]. It is not analytic at
the quantum critical point $h = 1$, as a trivial consequence of the non-analyticity of its building
blocks (i.e. $\epsilon$, $\Delta \phi$). However it is clear from the inset that such non-analyticity is so weak that
is unrealistic to say that the out-of-equilibrium behavior of entanglement entropy is sensitive
to the phase transition.

From Eq. (7.39) we also have the large time corrections to the asymptotic result. Since
$H(\pm 1) = 0$ with a log singularity, when the zero-velocity mode giving the large $t$ behavior is

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig7_1.png}
\caption{Speed of sound - R defined in Eq. (7.41) for quenches from ($h_0 = 10, \gamma_0 = 2$). The inset shows the singular behavior in the neighborhood of $h = 1$.}
\end{figure}
at $\varphi = \pm \pi$ (as e.g. for $h > 1$), one has that the first correction is $\propto \ell^4 \log t/t^3$, whereas when there are zero-velocities not at the border of the Brillouin zone, where $H(x)$ is finite, the leading correction is $\propto \ell^2/t$.

It is worth mentioning that from Eq. (7.39) it follows that for the quenches from $h_0 = \infty$ to any $|h| \leq 1$, all curves collapse on a single curve when rescaling $S(t)$ to $S(\infty)$. However this is only approximately true for strong magnetic fields ($|h| > 1$). For $t = \infty$ only the second term in Eq. (7.39) contributes to the entropy that thus is extensive, according to our previous interpretation of the late time behavior as a thermal state (or as a GGE). Moreover, the result is symmetric under the exchange $(h, \gamma) \leftrightarrow (h_0, \gamma_0)$, because Eq. (7.39) only depends on $\cos \Delta \varphi$ that does not distinguish between initial and final values.

The matrix representation (7.43) allows for the numerical calculation of $S(t)$ for finite and relatively large $\ell$. Some results are reported in Fig. 7.2 where we choose those quench parameters that make the finite $\ell$ effects more relevant. Increasing $\ell$ the results always approach Eq. (7.39), showing unambiguously its correctness, but there are peculiar and interesting finite $\ell$ effects. The most evident effect is the oscillation of $S(t)$, which can be present only when there is a second local maximum of $|\epsilon'|$. Data provide strong evidence that the first non-oscillating

![Figure 7.2: Quench dynamics](image-url)
correction at order $O(\ell^0)$ is positive and time independent.

In the bottom-left plot in Fig. 7.2 the most unexpected effect is shown. For the quench $(h_0 = 1, \gamma_0 = 0.4) \rightarrow (h = 0.5, \gamma = 0.2)$, it seems that the linear regime of $S_\ell(t)$ continues after $t^* = \ell/2\nu_M$. However, looking at the derivative (inset) one realizes that it is not exactly constant, since it slightly bends at $t^*$. This happens because for this peculiar quench the maximum velocity mode carries very little information, and so a stronger non-analyticity is present at a local maximum of the velocity smaller than $\nu_M$. This effect is pronounced every time that $h_0 \gamma \sim h_0 \gamma_0$, with $|h|, |\gamma|, |h_0|, |\gamma_0| < 1$, because of the functional form of $\Delta_\varphi$. This anomalous behavior is important because it is nowadays common to extract the speed of propagation of information from $t^*$. Every time this effect is present, this procedure gives the wrong answer. For example, we plotted in the inset of Fig. 7.2 the numerical derivative of $S_\ell(t)$ for $\ell = 90$ (a value hardly reached in non-equilibrium simulation). It is evident that at $t^*$ there is no trace of the non-analyticity. Relying on these results one would have obtained a value of $\nu_M$ that is almost half of the real one.

**Method.** As explained in Chapter 2, the entanglement entropy can be written in terms of a block Toeplitz matrix \[130\]. One first introduces the Majorana operators (2.35), namely $a_{2l-1} = (\prod_{m<l} \sigma_z^m) \sigma_x^l$ and $a_{2l} = (\prod_{m<l} \sigma_z^m) \sigma_y^l$, and the correlation matrix $\Gamma^A_\ell$ through the relation $\langle a_m a_n \rangle = \delta_{mn} + \Gamma^A_{mn}$ with $1 \leq m, n \leq \ell$, that is a block Toeplitz matrix $\Gamma^A_{ln} = \Gamma_{n-l}$, with

$$\Gamma_l = \begin{bmatrix} -f_l & g_l \\ -g_{-l} & f_{-l} \end{bmatrix},$$

and

$$g_l = -i \int_{-\pi}^{\pi} \frac{d\varphi}{2\pi} e^{-i\varphi l} e^{-i\theta_\varphi} (\cos \Delta_\varphi + i \sin \Delta_\varphi \cos 2\epsilon_\varphi t),$$

$$f_l = \int_{-\pi}^{\pi} \frac{d\varphi}{2\pi} e^{-i\varphi l} \sin \Delta_\varphi \sin 2\epsilon_\varphi t, \quad (7.42)$$

$$\cos \theta_\varphi = -(h - \cos \varphi)/\epsilon, \quad \text{and} \quad \sin \Delta_\varphi = -\sin \varphi [\gamma h_0 - \gamma_0 h - \cos (\gamma - \gamma_0)]/\epsilon \epsilon_0.$$ The entanglement entropy is given by

$$S_\ell = -\text{Tr} \left[ \frac{1}{2} \log \left( \frac{1 + \Gamma}{2} \right) \right]. \quad (7.43)$$

This trace can be worked out analytically by series expanding the function inside of the trace in powers of $\Gamma$. In this way we bring the problem to the determination of the asymptotic behavior of the trace of powers of block Toeplitz matrices. In Ref. \[12\] we have obtained the asymptotic behavior when the block Toeplitz matrix has a symbol that depends on time like the symbol of the correlation matrix after a quench in the XY model. However, we have given a proof too concise and slightly inaccurate. In the Appendix we provide a new proof. Here we report the result: the trace of the powers of the Toeplitz matrix

$$T_{ln} = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\varphi e^{-i(l-n)} \hat{\varphi}(\varphi) \quad (7.44)$$
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with symbol
\[ \hat{t}(\varphi) = n_x(\varphi)\sigma_x(\varphi) + n_\perp(\varphi) \cdot \tilde{\sigma}^{(\varphi)} e^{2i\epsilon(\varphi)\tau_3(\varphi)} \]
where \( \sigma_\alpha^{(\varphi)} = e^{-i\tilde{\theta}(\varphi)\cdot \sigma_\alpha e^{i\tilde{\theta}(\varphi)\cdot \varphi} } \) (7.45)

in the scaling limit \( t \sim \ell \) is given by
\[
\frac{1}{\ell} \text{Tr} \prod_{\ell > 1}^{2n} \int_{-\pi}^{\pi} \frac{d\varphi_0}{2\pi} \left( n_x(\varphi_0)^2 + n_\perp(\varphi_0)^2 \right)^n + \int_{2|\epsilon|<\ell} \frac{d\varphi_0}{2\pi} \frac{2|\epsilon'(\varphi_0)|}{\ell} \left[ n_x(\varphi_0)^{2n} - \left( n_x(\varphi_0)^2 + n_\perp(\varphi_0)^2 \right)^n \right] + \int_{2|\epsilon|>\ell} \frac{d\varphi_0}{2\pi} \left[ n_x(\varphi_0)^{2n} - \left( n_x(\varphi_0)^2 + n_\perp(\varphi_0)^2 \right)^n \right]. \tag{7.46}
\]

The trace of odd powers is subleading. Finally, Eq. (7.39) can be obtained by substituting the symbol of the block Toeplitz matrix \( \Gamma \) into Eq. (7.46) and summing the series expansion of Eq. (7.43).

Disjoint blocks. We now consider the evolution of R\'enyi entropies of disjoint blocks after a quench. We have seen that a connected spin block reacts to the quench increasing R\'enyi entropies linearly in time up to each spin in the subsystem becomes entangled with the environment. Then entropies saturate. The only relevant difference when the subsystem consists of two disjoint blocks is in the necessity to subtract the mutual entropy. However in Chapter 2 we have emphasized the differences between the spin and the fermionic representation. Our only goal here is to understand the differences between the two representations for the evolution after a quench. We only report the results shown in Ref. [9] where we have considered the R\'enyi entropy \( S_2 \). We compare the numerical data with the prediction that follows from the interpretation of the entanglement evolution in terms of motion of quasiparticles [15], described above. According to this physical scenario, for a general bipartition the result is

\[ S_\alpha(t) \approx \int_{x' \in A} dx' \int_{x'' \in B} dx'' \int_{-\infty}^{\infty} dx H_\alpha(p) dp \rho(x' - x - v(p)t) \delta(x'' - x - v(p)t), \tag{7.47} \]

where we assumed momentum conservation. For a double interval, this formula predicts a series of linear behaviors, with different slopes, that finally saturates at late time. The function \( H_\alpha \) does not depend on the subsystem length and topology. We derived it for a single interval [12]

\[ H_\alpha(\cos \Delta) = \frac{1}{1 - \alpha} \log \left[ \left( \frac{1 + \cos \Delta}{2} \right)^\alpha + \left( \frac{1 - \cos \Delta}{2} \right)^\alpha \right], \tag{7.48} \]

where \( \Delta(p) \) is the difference between the Bogoliubov angles before and after the quench. Thus, plugging everything together, the leading order of R\'enyi entropies is

\[ S_{\ell_1, r, \ell_2}(t) \sim S_{\ell_1}(t) + S_{\ell_2}(t) - \Delta S[\ell_1, r, \ell_2](t), \tag{7.49} \]

with \( (x_{\{a,b\}}(x) \equiv \theta(x-a)\theta(b-x)) \)

\[ \Delta S(t) = \int_{-\pi}^{\pi} \frac{d\varphi}{2\pi} H_\alpha(\cos \Delta) \int_{r}^{2|\epsilon'|} dv \left( \chi_{[r, r + \min(\ell_1, \ell_2)]}(v) - \chi_{[r + \max(\ell_1, \ell_2), r + \ell_1 + \ell_2]}(v) \right) \tag{7.50} \]
and

\[ S_\ell(t) = t \int_{2|\varepsilon'|t<\ell} \frac{d\varepsilon'}{2\pi} |\varepsilon'| H_\alpha(\cos \Delta) + \ell \int_{2|\varepsilon'|t>\ell} \frac{d\varepsilon'}{2\pi} H_\alpha(\cos \Delta). \]  

(7.51)

**Figure 7.3:** \(S_2\) for disjoint subsystems - Evolution of the Renyi entropy \(S_2\) after a global quench from a non critical system to a critical Ising. The asymptotic prediction is given by equation (7.49) while the fermionic entanglement is obtained neglecting the string contribution. When \(\{\Gamma_1, \Gamma_2\}\) becomes negligible with respect to \(\{\Gamma_1^2\}\), a jump of about \(\sim \log 2\) is seen. In the graph this happens in the neighborhood of the time \(t \sim 11\). The asymptotic prediction presents a small offset due to the finite entanglement in the initial state.

Let us now go back to the direct computation of the entanglement in two blocks after a quench Eq. (3.40). We observe that not all terms contribute to the leading order in the blocks’ lengths and distance: the string expectation value decays exponentially and only terms constructed with \(\Gamma_1\) and \(\Gamma_2\) survive. For instance the Renyi entropy \(S_2\) is simply the logarithm of two terms

\[ S_2 \sim -\log \left( \frac{1}{2} \exp \left( \frac{1}{2} \text{Tr} \log \frac{1+\Gamma_1^2}{2} \right) + \frac{1}{2} \exp \left( \frac{1}{2} \text{Tr} \log \frac{1+\Gamma_1 \Gamma_2}{2} \right) \right) \sim \begin{cases} -\frac{1}{2} \text{Tr} \log \frac{1+\Gamma_1^2}{2} + \log 2 + c & \text{Tr} \log \frac{1+\Gamma_1 \Gamma_2}{2} < \text{Tr} \log \frac{1+\Gamma_1^2}{2} \\ -\frac{1}{2} \text{Tr} \log \frac{1+\Gamma_1^2}{2} + c & \text{Tr} \log \frac{1+\Gamma_1 \Gamma_2}{2} \sim \text{Tr} \log \frac{1+\Gamma_1^2}{2} \\ -\frac{1}{2} \text{Tr} \log \frac{1+\Gamma_1 \Gamma_2}{2} + c + \log 2 & \text{otherwise} \end{cases} \]  

(7.52)

Analyzing several data (we report only a single example in Fig. 7.3), we deduce that in the scaling limit the term constructed with the standard fermionic correlations is never negligible: finite order Renyi entropies are controlled by fermionic correlations. When other terms are comparable with \(\{\Gamma_1, \cdots, \Gamma_1\}\), they give additive \(O(\ell^0)\) contribution of the form \(\sim \log k\), where \(k\) is the coefficient in front of the factor \(\{\cdots\}\), and \(k = 2\) for \(S_2\).
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The quasi-particle interpretation [15] perfectly agrees (up to a constant) with the fermionic representation $\rho_{\Gamma}$, (see Fig. 7.3). In other words the non locality of the Jordan-Wigner transformation does not influence (as one expects) the leading order of time evolution of entropies after a global quench. However, as in the non-critical equilibrium case, we observe an additive $\log 2$ contribution (in Fig. 7.3 a stick of width $\log 2$ is included to appreciate this difference) from the string and we believe that this is a general feature that will persist also away from criticality. As a final comment, we mention that the $O(\ell^0)$ offset of the numerical data at finite $\ell$ compared with the asymptotic form is a consequence of the initial entanglement. This subleading term is present also for the single interval case [12], and can be included in the asymptotic result [131].

In the next section we continue the analysis of the quench dynamics by considering the evolution of the order parameter in the Ising model.

7.2.2 Correlation functions

We now focus on the quench dynamics in the transverse field Ising chain. Although we have shown at the beginning that late time after a quench in the XY model (and hence in the Ising chain) the state does relax to a GGE regardless of the (local) observable under consideration, it was pointed out [116 132] that the locality, not intended here as spatial locality, of the observable with respect to the elementary excitations is expected to affect the time behaviour of an observable after a quantum quench. The order parameter is non-local with respect to the fermionic degrees of freedom, so it is an ideal testing ground for thermalization ideas. Here we present the results of Ref. [11], where we obtained analytical expressions for the full asymptotic time and distance dependence of one- and two-point correlation functions of the order parameter in the thermodynamic limit after a quantum quench within the ferromagnetic phase. We also present partial results for quenches within the paramagnetic phase and across the critical point. Our results have been obtained by two independent methods. The first is based on the determinant representation of correlation functions characteristic of free-fermionic theories. The second is based on the form-factor approach [133 134] and is applicable more generally to integrable quenches in interacting quantum field theories. This method complements existing analytical/semi-numerical methods used for studying quantum quenches in integrable systems [112 135 136 137 138], but has the advantage of providing analytic answers directly in the thermodynamic limit.

In fact we have found that at late times after a quench within the ordered phase ($h, h_0 \leq 1$) the order parameter $\rho_x \equiv \langle \sigma_x^z \rangle$ relaxes to zero exponentially fast

$$\rho_x(t) \propto \exp \left( t \int_0^{\pi} \frac{dk}{\pi} \varepsilon'_h(k) \ln (\cos \Delta_k) \right), \quad (7.53)$$

where $\varepsilon'_h(k) = d\varepsilon_h(k)/dk$. The two-point function of the order parameter exhibits exponential
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decay both in time and distance (\(\theta(x)\) denotes the Heaviside function)

\[
\rho^{xx}(\ell, t) \propto \exp \left[ t \int_0^\pi \frac{dk}{\pi} \ln (\cos \Delta_k) \theta(2\epsilon_h^\prime(k)t - \ell) \right] \\
\times \exp \left[ 2t \int_0^\pi \frac{dk}{\pi} \epsilon_h^\prime(k) \ln (\cos \Delta_k) \theta(\ell - 2\epsilon_h^\prime(k)t) \right].
\]

(7.54)

In the \(\ell \to \infty\) limit the first factor is equal to unity and \(\rho^{xx}(\infty, t) = (\rho^x(t))^2\), confirming cluster decomposition in our non-equilibrium situation. Fig. 7.4 shows a comparison of our asymptotic result for \(\rho^{xx}(\ell, t)\) to numerical data, establishing the accuracy of the former even for relatively short separations and times. We note that (7.54) holds even for quenches to or from the quantum critical point and agrees with the general form put forward in Ref. [16] on the basis of semiclassical arguments.

![Figure 7.4: Quench dynamics in the ordered phase](image)

Figure 7.4: Quench dynamics in the ordered phase - \(\rho^{xx}(\ell, t)\) for the quench \(h_0 = 0.3 \to h = 0.5\) at fixed distance \(\ell = 20\) and \(\ell = 40\) against the prediction in (7.54). The overall amplitude of \(\rho^{xx}\) has been used as the same fit parameter in both cases.

Surprisingly the decay time in (7.53) can be explained in terms of a GGE, even though it is not a property of the stationary state. The one point function (7.53) is characterized by exponential decay with rate \(\tau^{-1} = -\int_0^\pi \frac{dk}{\pi} \epsilon_h^\prime(k) \ln (\cos \Delta_k)\). This can be interpreted as the average mode-dependent decay time \(\tau^{-1}(k) = \epsilon_h^\prime(k)\xi^{-1}(k)\), obtained by multiplying the mode-dependent inverse correlation length by the velocity. The relaxational behaviour of the two-point function can be understood following [16] by rewriting (7.54) as

\[
\frac{\rho^{xx}(\ell, t)}{(\rho^x(t))^2} \sim \exp \left[ \int_0^\pi \frac{dk}{\pi} \left( \frac{\ell}{\xi(k)} - \frac{2t}{\tau(k)} \right) \theta(2\epsilon_h^\prime(k)t - \ell) \right].
\]

(7.55)
The theta-function expresses the fact that a given mode can only contribute to the relaxational behaviour if the distance \( \ell \) lies within its forward “light cone”, while the form of the remaining factor follows from the known stationary behaviour. And analogous conclusions can be drawn for the entanglement entropy Eq. (7.39).

We stress that the momenta responsible for the slow-decay of the interaction in the entanglement Hamiltonian (7.37) do not contribute to the one- and two-point correlation functions, as well as to the entanglement entropy, indeed \( \log \cos \Delta = 0 \) and \( H(\cos \Delta) = 0 \) when \( \cos \Delta = \pm 1 \).

This is not true anymore considering e.g. the magnetization along the direction of the magnetic field, which is instead a local operator with respect to the elementary excitations. However the relation between the two phenomena has not been yet investigated.

Figure 7.5: Ordered to disordered - The ratio \( \rho_{xx}(\ell,t)/\rho_{xx}^{\text{asymp}}(t) \), where \( \rho_{xx}^{\text{asymp}}(t) \) is the exponential decay in Eq. (7.56), for the quench \( h_0 = 0 \rightarrow h = 3 \) at fixed distance \( \ell = 30 \) against the oscillating function in Eq. (7.56).

In the disordered phase the behaviour of correlation functions of \( \sigma^x \) is more involved \[139\] \[140\]. The simplest case is of quenches from the ordered to the disordered phase. Semi-analytic arguments suggest the following behavior of the two-point correlation function for times \( t < \frac{\ell}{2v_{\text{max}}} \) :

\[
\rho_{xx}(\ell,t) \propto \cos^2(\varepsilon_h(0)(t + \delta t)) \exp\left[\int_0^\pi \frac{dk}{\pi} \ln(\cos \Delta_k) 2\varepsilon'_h(k) t\right],
\] (7.56)

with \( \delta t \) a parameter independent of time (see Fig. 7.5), whilst for larger times the period of oscillations increases and their amplitude decreases to finally disappear. In spite of these complications, the correlation length characterizing the stationary behaviour of \( \rho_{xx}(\ell,t = \infty) \sim \exp(-\ell/\xi) \) for an arbitrary quench can be cast in the simple form

\[
\xi^{-1} = \theta(h - 1)\theta(h_0 - 1) \ln(\min[h_0, h_1]) - \ln \left[ x_+ + x_- + \theta((h - 1)(h_0 - 1)) \sqrt{4x_+ x_-} \right],
\] (7.57)
where $x_\pm = \frac{1}{2} [\min(h, h^{-1}) \pm 1][\min(h_0, h_0^{-1}) \pm 1]$ and $h_1 = \frac{1 + h_{0} + \sqrt{(h^2 - 1)(b_0^2 - 1)}}{h + h_{0}}$.

**Method I: Determinant approach.** We focus on the two-point function $g^{zz}(\ell, t)$, which can be written as the determinant of a $2\ell \times 2\ell$ block Toeplitz matrix $T$. The matrix elements of $T$ depend explicitly on the time $t$. In the stationary state the $t$ dependence disappears and the large-$\ell$ behaviour can be obtained by application of the generalized Szego lemma [144], resulting in (7.57). The dynamics in the limit $t, \ell \to \infty$ at fixed ratio $t/\ell$ is much more difficult to determine, as the elements of $T$ then depend on the matrix dimension itself and Szego’s lemma does not apply. To deal with this situation we employ a method similar to [12]. In order to calculate $\ln \det |T| = \text{Tr} \ln |T|$, we consider the moments of $T$, i.e. $\text{Tr} T^{2n}$ (we find that odd moments are subleading). Calculating these moments gives (see the Appendix)

$$\text{Tr} T^{2n} = \ell \int_{-\pi}^{\pi} \frac{dk}{2\pi} (\cos \Delta_k)^{2n} + \int_{-\pi}^{\pi} \frac{dk}{2\pi} \varepsilon (\ell - 2|\varepsilon_k'(k)|t) \left[ 1 - \left( \cos \Delta_k \right)^{2n} \right], \quad (7.58)$$

where $\varepsilon(x) = x\theta(x)$. The trace of any analytic function $f$ of $T$ can be formally expanded in the moments. In our case we are interested in $f(x) = \ln |x|$, which is analytic in the principal strip for any $x \neq 0$. As the symbol of the block Toeplitz matrix has winding number zero about the origin and $\cos(\Delta_k)$ is always non zero we can resum the expansion of the logarithm to obtain (7.54).

**Method II: Form-factor approach.** This approach applies more generally to quenches in integrable (interacting) quantum field theories. We focus on the 1-point function in the ordered phase. The ground state for $|h| < 1$ spontaneously breaks the $\mathbb{Z}_2$ symmetry of the TFIC, resulting in an initial (ground) state of the form

$$|\Omega\rangle = \frac{1}{\sqrt{2}} \left[ |B\rangle_{R} + |B\rangle_{NS} \right], \quad (7.59)$$

where R and NS refer to the periodic/antiperiodic sectors of the free-fermion theory respectively and e.g. $|B\rangle_{R} = \exp \left( i \sum_{\sigma < \rho \in \mathbb{R}} K(p) b_{\sigma}^\dagger b_{\rho} \right) |0\rangle_{R}$, where $K(p) = \tan(\Delta_p/2)$ and $b_p^\dagger$ is a fermion creation operator with momentum $p$. The 1-point function is

$$\frac{\langle \Omega | \sigma_m^z(t) | \Omega \rangle}{\langle \Omega | \Omega \rangle} = 2 \frac{\text{NS} \langle B | \sigma_m^z(t) | B \rangle_{R}}{\text{NS} \langle B | B \rangle_{NS} + \text{R} \langle B | B \rangle_{R}}. \quad (7.60)$$

Expanding the “boundary states” $|B\rangle_{R,NS}$ results in a Lehmann representation for (7.60). Crucially, the matrix elements (form factors) of $\sigma_m^z(t)$ between multifermion Hamiltonian eigenstates are known exactly for the TFIC [145]. The main idea for evaluating the Lehmann representation then follows the finite temperature case [146,147,148,149,150]. For a small quench the (total) density $n_0$ of fermion excitations in the initial state constitutes a small parameter. In this case one can use the $K(k)$-matrix as an expansion parameter. One then observes that the form factors appearing in the Lehmann representation are singular when momenta in the in and out states coincide. The leading (in the density $n_0$) contribution to the one point function is obtained by summing all terms with the strongest singularities at a given order in the expansion.
in powers of $K$. This amounts to the exponentiation of infrared singularities. We note that just as in the finite temperature case infinite volume divergences encountered in evaluating the numerator of (7.60) cancel against analogous divergencies in the denominator. The result of these calculations is

$$\langle \Omega | \sigma_m^z(t) | \Omega \rangle \propto \exp \left[ -t \int_0^\pi \frac{dk}{\pi} K^2(k) 2e'(k) \right].$$  \hspace{1cm} (7.61)

The decay rate agrees with the leading term in the expansion of (7.53) in powers of $K^2(k)$. The correction to the $K^2(k)$ factor in (7.61) are found to be $O(K^6)$, again in agreement with (7.53). We note that (7.61) provides an excellent approximation to (7.53) as long as $h, h_0$ are not too close to the critical point. The two-point function can be analyzed in an analogous manner and the results again agree with the appropriate expansion of (7.54). Things become more complicated considering quenches in the disordered phase, because it becomes difficult, if not impossible, to guess the structure of all pieces of the form-factor expansion in order to resum the series. Nevertheless, this approach could be preferable with respect to the first method, providing at least approximate results, which become more and more precise as the smaller is the quench ($|\cos \Delta| - 1 \ll 1$)

In this chapter we introduced the concept of quantum quench. We discussed the problem of relaxation focusing in particular on the role played by conservation laws. In most cases the late time behavior in non-integrable models can be described in terms of an effective temperature. On the other hand, in integrable models the memory of the initial state can not be retained in a single parameter (the temperature), since there are infinite conservation laws. Then, we reviewed the CFT results on the evolution of one- and two-point correlation functions of primary fields as well as of the entanglement entropy. Finally, we reported the results of Refs. [12] and [13], in which we obtained the analytical expressions for the evolution after a quantum quench within the XY model both for correlation functions and for the entanglement in the scaling limit $\ell \sim t \gg 1$. 

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Appendix A. Trace of integer powers of block Toeplitz matrices

In this appendix we consider the trace of the power \( n \) of the block-Toeplitz matrix

\[
T \equiv \frac{1}{2\pi} \int_{-\pi}^{\pi} d\varphi e^{-i(l-n)\varphi} \hat{t}(\varphi). \tag{A.1}
\]

\( \hat{t}(\varphi) \) is a 2-by-2 matrix that can be then written in terms of Pauli matrices. We consider those matrices of the form

\[
\hat{t}(\varphi) = n_x(\varphi)\sigma_x(\varphi) + \vec{n}_\perp(\varphi) \cdot \vec{\sigma} e^{2i\varphi_0(\varphi)\sigma_z(\varphi)}. \tag{A.2}
\]

where \( t \) is the only parameter comparable with the matrix size \( \ell \), and we leave the possibility of a local rotation of the Pauli matrices

\[
\sigma_\alpha(\varphi) \sim e^{-i\vec{\theta}(\varphi) \cdot \vec{\sigma}} e^{i\vec{\theta}(\varphi) \cdot \vec{\sigma}}. \tag{A.3}
\]

For example, the symbol corresponding to a quench in the XY model is

\[
n_x(\varphi) = \cos \Delta \quad \text{and} \quad \vec{n}_\perp = (0, 0, \sin \Delta), \]

where \( \Delta = \theta - \theta_0 \) is the difference between the Bogoliubov angles of the final and initial Hamiltonian. The rotation parameter \( \theta_\varphi \) in Eq. (A.3) is just the Bogoliubov angle of the final Hamiltonian. When evaluating \( \text{Tr}[T^n] \), each multiplication of two consecutive matrices involves a sum over the indices, that can be put in integral form by means of the identity

\[
\sum_{j=1}^{\ell} e^{-i(j-\frac{\ell+1}{2})\varphi} = \frac{\ell}{2} \int_{-1}^{1} d\xi \frac{\varphi}{2\sin(\xi)} e^{it\xi \varphi}. \tag{A.4}
\]

Using this expression, after some algebraic manipulations, we get

\[
\text{Tr}[T^n] = \left( \frac{\ell}{2} \right)^n \int_{[-\pi,\pi]^n} \frac{d^n\varphi}{(2\pi)^n} \int_{[-1,1]^n} d^n\xi \prod_{i=0}^{n-1} \frac{\varphi_i - \varphi_{i-1}}{2\sin(\frac{\varphi_i - \varphi_{i-1}}{2})} e^{i\ell \sum_{j=0}^{n-1} \xi_i \varphi_{i+1} - \xi_i \varphi_i} \times \]

\[
\text{Tr} \left[ \prod_{i=0}^{n-1} n_x(\varphi_i)\sigma_x(\varphi_i) + \vec{n}_\perp(\varphi_i) \cdot \vec{\sigma} e^{2i\varphi_0(\varphi)\sigma_z(\varphi_i)} \right], \tag{A.5}
\]

where we introduced \( \varepsilon_i = \varepsilon(\varphi_i) \). By changing variables

\[
\begin{cases}
\xi_0 = \xi_\frac{1}{2} \\
\xi_i = \xi_{i+1} - \xi_i \quad i \in [1, n-1]
\end{cases}
\]

(A.6)
We interpret the resulting integration as a functional $\hat{\mu}$ the previous expression becomes

$$
\text{Tr} T^n = \left( \frac{\ell}{2} \right)^n \int_{[-\pi, \pi]^n} \frac{d^n \varphi}{(2\pi)^n} \int d^n \zeta \prod_{i=0}^{n-1} \varphi_i - \varphi_{i-1} 2 \sin \left( \frac{\varphi_i - \varphi_{i-1}}{2} \right) e^{-\imath \sum_{j=1}^{n-1} \zeta_j \frac{\varphi_j - \varphi_0}{\pi}} \times \text{Tr} \left[ \prod_{i=0}^{n-1} n_x (\varphi_i) \sigma_x^{(\varphi)} + \vec{n}_\perp (\varphi_i) \cdot \vec{\sigma}(\varphi) e^{2\imath \epsilon_i i \sigma_z^{(\varphi)}} \right],
$$

(A.7)

where the domain of integration $R_\zeta$ is determined by the conditions

$$
-1 \leq \sum_{j=0}^{k-1} \zeta_j \leq 1 \quad \forall k \in [1, n].
$$

(A.8)

The integrand does not depend on $\zeta_0$, and hence we can perform the integral in this variable

$$
\text{Tr} T^n = \left( \frac{\ell}{2} \right)^n \int_{[-\pi, \pi]^n} \frac{d^n \varphi}{(2\pi)^n} \int d^n \zeta \mu(\vec{\zeta}) \prod_{i=0}^{n-1} \varphi_i - \varphi_{i-1} 2 \sin \left( \frac{\varphi_i - \varphi_{i-1}}{2} \right) e^{-\imath \sum_{j=1}^{n-1} \zeta_j \frac{\varphi_j - \varphi_0}{\pi}} \times \text{Tr} \left[ \prod_{i=0}^{n-1} n_x (\varphi_i) \sigma_x^{(\varphi)} + \vec{n}_\perp (\varphi_i) \cdot \vec{\sigma}(\varphi) e^{2\imath \epsilon_i i \sigma_z^{(\varphi)}} \right],
$$

(A.9)

with

$$
\mu(\vec{\zeta}) = \max \left[ 0, \min_{j \in \{0, n-1\}} \left[ 1 - \sum_{k=1}^{j} \zeta_k \right] + \min_{j \in \{0, n-1\}} \left[ 1 + \sum_{k=1}^{j} \zeta_k \right] \right].
$$

(A.10)

We interpret the resulting integration as a functional $\hat{I}_n$ that applies to the symbol

$$
\hat{I}_n^{(i)} f \equiv \left( \frac{\ell}{2} \right)^n \int_{[-\pi, \pi]^n} d^n \varphi \int d^n \zeta \mu(\vec{\zeta}) \prod_{i=0}^{n-1} \varphi_i - \varphi_{i-1} 2 \sin \left( \frac{\varphi_i - \varphi_{i-1}}{2} \right) e^{-\imath \sum_{j=1}^{n-1} \zeta_j \frac{\varphi_j - \varphi_0}{\pi}} f(\varphi_0, \ldots, \varphi_{n-1}) .
$$

(A.11)

We study the asymptotic limit $\ell \to \infty$ using a multi-dimensional phase approximation. Because the symbol is independent of the integration variables $\zeta_i$, by asking for the stationarity of these variables we get the constraint

$$
\varphi_j \approx \varphi_0 \quad \forall j \in [1, n-1] .
$$

(A.12)

Thus we can substitute any variable $\varphi_j$ with $\varphi_0$ as long as it does not appear in rapidly oscillating terms, let us call this the localization rule

$$
\hat{I}_n \xrightarrow{\ell \to \infty} \left( \frac{\ell}{2} \right)^n \int_{[-\pi, \pi]^n} d^n \varphi \mu(\vec{\varphi}) e^{-\imath \sum_{j=1}^{n-1} \varphi_j \frac{\varphi_j - \varphi_0}{\pi}} .
$$

(A.13)

Because of the functional form of $\mu(\vec{\zeta})$ in Eq. (A.10), when $\hat{I}_n$ is applied to a function that does not depend on all the variables

$$
f(\varphi_0, \ldots, \varphi_{n-1}) = \hat{f}(\varphi_{j_1}, \ldots, \varphi_{j_k}) \quad 0 \leq j_1 < j_2 < \cdots < j_k < n - 1
$$

(A.14)
the result is independent of the particular ordered sequence \( \{j_1, \cdots, j_k\} \)

\[
\tilde{f}(\varphi_{j_1}, \cdots, \varphi_{j_k}) \sim \tilde{f}(\varphi_0, \cdots, \varphi_{k-1}). \tag{A.15}
\]

We call this property the contraction rule. We now apply the two rules to the Toeplitz symbol. The localization rule allows the substitution of the integration variable in \( n_x \) and \( \vec{n}_\perp \), and the cancellation of the local rotation of the Pauli matrices

\[
f(\varphi_0, \cdots, \varphi_{n-1}) = \Tr \left[ \prod_{i=0}^{n-1} \left( \frac{1 + \tau_i}{2} n_x(\varphi_0)\sigma_x + \frac{1 - \tau_i}{2} \vec{n}_\perp(\varphi_0) \cdot \vec{\sigma} e^{2i \varepsilon_s t \sigma_s} \right) \right]. \tag{A.16}
\]

By transforming this product into a sum over the configurations of the classical variables \( \tau_i \in \{-1, 1\} \)

\[
f(\varphi_0, \cdots, \varphi_{n-1}) = \sum_{\{\tau\}} \Tr \left[ e^{-\sum_{j=0}^{n-1} \frac{1-\tau_j}{2} \sum_{k=0}^{j-1} \tau_k 2i \varepsilon_s t \sigma_x} \prod_{i=0}^{n-1} \left( \frac{1 + \tau_i}{2} n_x(\varphi_0)\sigma_x + \frac{1 - \tau_i}{2} \vec{n}_\perp(\varphi_0) \cdot \vec{\sigma} \right) \right]. \tag{A.17}
\]

we can move the exponentials to the left taking care of the change in sign

\[
f(\varphi_0, \cdots, \varphi_{n-1}) = \sum_{\{\tau\}} \Tr \left[ e^{-\sum_{j=0}^{n-1} \frac{1-\tau_j}{2} \sum_{k=0}^{j-1} \tau_k 2i \varepsilon_s t \sigma_x} \prod_{i=0}^{n-1} \left( \frac{1 + \tau_i}{2} n_x(\varphi_0)\sigma_x + \frac{1 - \tau_i}{2} \vec{n}_\perp(\varphi_0) \cdot \vec{\sigma} \right) \right]. \tag{A.18}
\]

We expand the exponential in trigonometric functions (in the following \( f(\varphi_0, \cdots, \varphi_{n-1}) \) is understood in front of \( = \))

\[
= \sum_{\{\tau\}} \cos \left( \sum_{j=0}^{n-1} \frac{1-\tau_j}{2} \sum_{k=0}^{j-1} \tau_k 2i \varepsilon_s t \right) \Tr \left[ \prod_{i=0}^{n-1} \left( \frac{1 + \tau_i}{2} n_x(\varphi_0)\sigma_x + \frac{1 - \tau_i}{2} \vec{n}_\perp(\varphi_0) \cdot \vec{\sigma} \right) \right] - \\
- \sum_{\{\tau\}} \sin \left( \sum_{j=0}^{n-1} \frac{1-\tau_j}{2} \sum_{k=0}^{j-1} \tau_k 2i \varepsilon_s t \right) \Tr \sigma_x \left[ \prod_{i=0}^{n-1} \left( \frac{1 + \tau_i}{2} n_x(\varphi_0)\sigma_x + \frac{1 - \tau_i}{2} \vec{n}_\perp(\varphi_0) \cdot \vec{\sigma} \right) \right]. \tag{A.19}
\]

and we rearrange the sum over the configurations, isolating a sum over the number of \( n_\perp \). In fact from the contraction rule it follows

\[
= \sum_{k=0}^{n} \cos \left( \sum_{j=0}^{k-1} (-1)^j 2i \varepsilon_s t \right) n_x(\varphi_0)^{n-k} n_\perp(\varphi_0)^k \frac{1}{k!} \frac{\partial^k}{\partial s^k} \left. \Tr(\sigma_x + s\sigma_y)^n \right|_{s=0} - \\
- \sum_{k=0}^{n} \sin \left( \sum_{j=0}^{k-1} (-1)^j 2i \varepsilon_s t \right) n_x(\varphi_0)^{n-k} n_\perp(\varphi_0)^k \frac{1}{k!} \frac{\partial^k}{\partial s^k} \left. \Tr(\sigma_x + s\sigma_y)^{n+1} \right|_{s=0} \tag{A.20}
\]

The traces can be easily evaluated

\[
\frac{1}{k!} \frac{\partial^k}{\partial s^k} \left. \Tr(\sigma_x + s\sigma_y)^n \right|_{s=0} = \frac{1}{k!} \frac{\partial^k}{\partial s^k} (1 + s^2)^n (1 + (-1)^n) \bigg|_{s=0} = \begin{cases} 2^{(n/2)} & n, k \text{ even} \\ 0 & \text{otherwise} \end{cases} \tag{A.21}
\]
A. TRACE OF INTEGER POWERS OF BLOCK TOEPLITZ MATRICES

and we get the result

\[ \sum_{k=0}^{\lfloor n/2 \rfloor} \left( \begin{array}{c} \lfloor n/2 \rfloor \\ k \end{array} \right) \left[ \exp \left( -i \sum_{j=0}^{2k-1} (-1)^j 2 \varepsilon_j t \right) + (-1)^n \exp \left( i \sum_{j=0}^{2k-1} (-1)^j 2 \varepsilon_j t \right) \right] n_x^{n-2k} \bar{n}_x^{2k}, \]  
\]

(A.22)

where \( n_x = n_x(\varphi_0) \) and \( \bar{n}_x(\varphi_0) \). Putting all together, because the phases in the expression above vanish at the stationary point, the odd powers are sub-leading (the asymptotic phase approximation gives 0) with respect to the even ones, and we find

\[ \text{Tr} T^{2n} \xrightarrow{\ell \to \infty} \ell \left( \frac{\ell}{2} \right)^{2n-1} \sum_{k=0}^{\lfloor n/2 \rfloor} \left( \begin{array}{c} n \\ k \end{array} \right) \int_{-\pi}^{\pi} \frac{d^{2n} \varphi}{(2\pi)^{2n}} \int d^{2n-1} \zeta n_x^{2n-2k} \bar{n}_x^{2k} \mu(\zeta) e^{-i \pi/2 \sum_{j=1}^{2n-1} \zeta_j x_j - \pi/2 + 2i \pi \sum_{j=0}^{2k-1} (-1)^j \varepsilon_j}, \]

(A.23)

We isolate the integration in \( \varphi_0 \)

\[ \text{Tr} T^{2n} \xrightarrow{\ell \to \infty} \ell \left( \frac{\ell}{2} \right)^{2n-1} \sum_{k=0}^{\lfloor n/2 \rfloor} \left( \begin{array}{c} n \\ k \end{array} \right) \int_{-\pi}^{\pi} \frac{d\varphi_0}{2\pi} n_x(\varphi_0)^{2n-2k} \bar{n}_x(\varphi_0)^{2k} \Lambda_{n;k}(\varphi_0), \]

(A.24)

with

\[ \Lambda_{n;k}(\varphi_0) = \int_{-\pi}^{\pi} \frac{d^{2n-1} \varphi}{(2\pi)^{2n}} \int d^{2n-1} \zeta \mu(\zeta) e^{-i \pi/2 \sum_{j=1}^{2n-1} \zeta_j x_j - \pi/2 + 2i \pi \sum_{j=0}^{2k-1} (-1)^j \varepsilon_j}, \]

(A.25)

and we apply the multi-dimensional phase approximation to \( \Lambda_{n;k}(\varphi_0) \). Remind the asymptotic result \[51\]

\[ \int_D d^n x g(x) e^{itf(x)} \xrightarrow{\ell \to \infty} \left( \frac{2\pi}{\ell} \right)^{n/2} \left( \frac{2\pi}{\ell} \right)^{-n/2} \left( \frac{2\pi}{\ell} \right)^{1/2} g(x_0) \det A^{-1} \exp \left( \frac{i\pi a}{4} \right), \]

(A.26)

where \( x_0 \) is a non-degenerate stationary point, \( A_{ij} = \partial_{x_i} \partial_{x_j} f(x_0) \) is the Hessian matrix of \( f \), and \( \sigma \) is the signature of the matrix \( A \), i.e. the difference between positive and negative eigenvalues. The stationary conditions are

\[ \begin{cases} \varphi_j = \varphi_0 & j = 1, \ldots, 2n - 1 \\ \zeta_j = 4^j (-1)^j \varepsilon_j & j = 1, \ldots, 2k - 1 \\ \zeta_j = 0 & j = 2k, \ldots, 2n - 1 \end{cases} \]

(A.27)

By ordering the variables such that the \( \zeta \)'s come before the \( \varphi \)'s, the Hessian assumes the following form

\[ A = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & M \end{pmatrix}, \]

(A.28)

and any eigenvalue \( a \) of \( A \) is in the simple relation with the eigenvalues \( \mu \) of the matrix \( M \)

\[ a_{\pm} = \mu \pm \sqrt{\mu^2 + 4}. \]

(A.29)
Thus the signature of $A$ is zero and the determinant is $-4^{1-2n}$. As previously anticipated, at the stationary point the phase in the integral vanishes because there is an even number of $\varepsilon$'s with alternating sign. The last step is to write $\mu(\zeta)$ Eq. (A.10) at the stationary point. We find

$$
\mu = \begin{cases} 
\frac{2}{7} \max[0, \ell - 2|\varepsilon'(\varphi_0)t|] & k \neq 0 \\
2 & k = 0.
\end{cases}
$$

(A.30)

Thus we get the final result

$$
\frac{1}{\ell} \text{Tr} g T^{2n} \overset{\ell \to 1}{\longrightarrow} \int_{-\pi}^{\pi} \frac{d\varphi_0}{2\pi} \left( n_\perp(\varphi_0)^2 + n_\perp(\varphi_0)^2 \right)^n + \\
\int_{2|\varepsilon'|t<\ell} \frac{d\varphi_0}{2\pi} \left( \frac{2|\varepsilon'(\varphi_0)t|}{\ell} \right)^n \left[ n_\perp(\varphi_0)^2 - \left( n_\perp(\varphi_0)^2 + n_\perp(\varphi_0)^2 \right)^n \right] + \\
+ \int_{2|\varepsilon'|t>\ell} \frac{d\varphi_0}{2\pi} \left[ n_\perp(\varphi_0)^2 - \left( n_\perp(\varphi_0)^2 + n_\perp(\varphi_0)^2 \right)^n \right].
$$

(A.31)

This formula gives the asymptotic behavior of the trace of any analytic function $g$ applied to $T$

$$
\frac{1}{\ell} \text{Tr} g(T) \overset{\ell \to 1}{\longrightarrow} \int_{-\pi}^{\pi} \frac{d\varphi_0}{2\pi} g_e \left( \sqrt{n_\perp(\varphi_0)^2 + n_\perp(\varphi_0)^2} \right) + \\
\int_{2|\varepsilon'|t<\ell} \frac{d\varphi_0}{2\pi} \left( \frac{2|\varepsilon'(\varphi_0)t|}{\ell} \right)^n \left[ g_e \left( n_\perp(\varphi_0) \right) - g_e \left( \sqrt{n_\perp(\varphi_0)^2 + n_\perp(\varphi_0)^2} \right) \right] + \\
+ \int_{2|\varepsilon'|t>\ell} \frac{d\varphi_0}{2\pi} \left[ g_e \left( n_\perp(\varphi_0) \right) - g_e \left( \sqrt{n_\perp(\varphi_0)^2 + n_\perp(\varphi_0)^2} \right) \right],
$$

(A.32)

where

$$
g_e(\varphi) = \frac{g(\varphi) + g(-\varphi)}{2}. \quad (A.33)
$$

The structure of the result suggests that the condition of $g$ to be analytic in a region enclosing every eigenvalue of $T$ could be substituted by the weaker (and verifiable) condition of analyticity on the images of $[-\pi, \pi]$ under the functions $n_\perp(\varphi)$ and $\sqrt{n_\perp(\varphi)^2 + n_\perp(\varphi)^2}$. This observation opens the way for a generalization of the Szegő lemma for the kind of time dependent symbols of Eq. (A.2). In particular we claim that, if the symbol at any time satisfies the Szegő hypotheses (in particular it has zero winding number), then

$$
\log \det T[\hat{t}] = \log \det T[\hat{t}_0] - (\log \det)_T T[\hat{t}_0] + (\log \det)_T T[\hat{t}_\infty], \quad (A.34)
$$

where the $(\log \det)_T$ functional can be obtained from the Szegő lemma by the substitution

$$
\int_{-\pi}^{\pi} \frac{d\varphi_0}{2\pi} \overset{\ell \to 1}{\longrightarrow} \int_{2|\varepsilon'|t<\ell} \frac{d\varphi_0}{2\pi} \left( \frac{2|\varepsilon'(\varphi_0)t|}{\ell} \right)^n + \int_{2|\varepsilon'|t>\ell} \frac{d\varphi_0}{2\pi}. \quad (A.35)
$$

In Ref. [13] we have used this conjecture to determine the asymptotic behavior of the evolution of the order parameter $((\sigma^f \sigma^r_{t+n}))$ in the scaling limit $t \sim n$, where $t$ is the time after a quench.
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in the Ising model. In particular we checked its correctness when the symbol has zero winding number, however the formula above is unable to capture the asymptotic behavior when the winding number is different from 0.
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