

Faculté des sciences

Quantum entanglement in inhomogeneous one-dimensional systems

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Chapter 1

Introduction

Quantum entanglement is one of the most intriguing features of quantum mechanics, yet one of the most fundamental. This phenomenon reveals that a measurement on some parts of a quantum system can influence the state of the other parts instantaneously and no matter how far apart they are in space. The story of entanglement starts in 1935 with Einstein, Poldolsky, and Rosen’s thought experiment, famously known as the EPR paradox [1]. The authors originally thought that their discovery showed an incompleteness of the theory of quantum mechanics. Around the same time, Schrödinger also studied that phenomenon, which he himself named entanglement [2].

To illustrate this concept, we consider a system composed of two electrons, A and B. We are interested in the spin of the electrons. Each electron is either in a state with its spin up, $|\uparrow^i\rangle$, or down, $|\downarrow^i\rangle$, where $i = A, B$. A possible state to describe our system of two electrons is

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle), \quad (1.1)$$

where $|ab\rangle = |a^A\rangle \otimes |b^B\rangle$ and $a, b \in \{\uparrow, \downarrow\}$. Let us consider two observers: Alice, who observes A, and Bob, who observes B. If Alice measures her spin in the state $|\uparrow^A\rangle$, she knows, from the axioms of quantum mechanics, that the system has collapsed to the state $|\downarrow\uparrow\rangle$. Hence, she knows instantaneously and certainly that the outcome of Bob’s measurement will be $|\downarrow^B\rangle$. This remains true even if the electrons are far apart. The instantaneity and spatial distance led Einstein and his collaborators to believe the phenomenon was in contradiction with the principles of Relativity.

It was not until 1964 that the weak point of the EPR paradox was discovered by John Bell with the so-called Bell’s inequality [3]. He argued that entanglement was actually compatible with the theory of quantum mechanics. Bell’s inequality was later proven experimentally by Aspect’s experiment [4, 5], which led to the 2022 Nobel Prize in Physics shared with Clauser and Zeilinger. Quantum entanglement has been widely studied ever since its introduction. It has found application in various research areas in physics, such as black hole physics [6], quantum information and quantum computing [7] or quantum optics [8].

In this thesis, we are interested in the study of entanglement in condensed matter models. This area of physics aims to describe systems with a large number of constituents in interactions. Entanglement plays a crucial role in the description of

such models. For instance, it is possible to detect and characterise quantum phase transitions in systems by studying their entanglement [9, 10].

This thesis is organised as follows. In **Chapter 2**, we review the concept of entanglement in quantum systems. In particular, we are interested in two different measures of entanglement, namely the so-called entanglement entropy and the so-called bipartite fidelity.

Chapter 3 is dedicated to the study of one-dimensional spin systems, called free-fermion models. We consider systems with inhomogeneous interactions. For such models, it is possible to diagonalise the Hamiltonian and thus explicitly construct the eigenstates of the system. In the diagonalisation process, we notice that free-fermion models share similarities with discrete orthogonal polynomials. This observation allows us to construct free-fermion models based on families of discrete orthogonal polynomials.

In the next two chapters, we apply the formalism constructed in Chapter 3 to two different sets of polynomials. In **Chapter 4**, we consider the Chebyshev polynomials of the second kind and recover the so-called homogeneous XX model. We first study the entanglement entropy in the ground state and in the first excited state of the system. Then, we study the bipartite fidelity in the ground state. We also expand this discussion by considering the first excited state. For both quantities, we compare our numerical results with known results.

In **Chapter 5**, we consider an inhomogeneous model based on the Krawtchouk polynomials. We first review some properties of these polynomials and then start our investigations of the entanglement in the ground state. For the entropy, we compare our numerical results with some known conjectures. For some choices of parameters, we notice that the ends of the chain are not entangled with the rest of it. This particular feature is investigated with the so-called local fermion density. We then move on to the study of the bipartite fidelity. The definition of this quantity is adapted to allow its study in an inhomogeneous model.

The numerical simulations presented in this work were all made using `python`. We always use the function `optimize.curve_fit` from the package `scipy` to fit our numerical results. Through the whole text, the results from the fits are presented as follows: $a \pm \sigma$ where a is the coefficient computed from the fit and σ is the order of the standard deviation for a . We round up a after the order of the standard deviation. If the order is larger than 10^{-4} , we round up after four decimal places.

Chapter 2

Entanglement in quantum systems

The aim of this chapter is to introduce the concept of entanglement in quantum systems. In particular, we focus on bipartite systems. There exist multiple ways to quantify and describe the entanglement in a quantum system [11, 12, 13]. We investigate two of them, namely, the so-called entanglement entropy and the so-called bipartite fidelity.

Let us first define entanglement. We consider a bipartite quantum system composed of two distinguishable subsystems, A and B . Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be the Hilbert spaces of the respective subsystems. We suppose that the Hilbert spaces are both finite-dimensional, with $\dim \mathcal{H}_A = n_A$ and $\dim \mathcal{H}_B = n_B$. The Hilbert space of the composite system is given by the tensor product $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$.

We consider a normalised state of the composite system $|\psi\rangle \in \mathcal{H}$. We say that the state is not entangled if it can be written as a tensor product of the states of the subsystems:

$$|\psi\rangle = |\psi^A\rangle \otimes |\psi^B\rangle. \quad (2.1)$$

Conversely, if this decomposition is not possible, we say the state is entangled. For instance, the state (1.1) is an entangled state, whereas the state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\uparrow\uparrow\rangle) = \frac{1}{\sqrt{2}}|\uparrow^A\rangle \otimes (|\downarrow^B\rangle + |\uparrow^B\rangle), \quad (2.2)$$

is not entangled.

2.1 Entanglement entropy

The first quantity we present is the entanglement entropy. We suppose that the bipartite system is in the normalised pure state $|\psi\rangle \in \mathcal{H}$, that is, it is described by a single wave function with probability one. Note that even if the composite system is in a pure state, that is not necessarily the case for the subsystems.

According to the Schmidt decomposition [7], there always exist two orthonormal bases, $\{|\varphi_i^A\rangle \in \mathcal{H}_A\}_{i=1}^{n_A}$ and $\{|\phi_i^B\rangle \in \mathcal{H}_B\}_{i=1}^{n_B}$, such that

$$|\psi\rangle = \sum_{i=1}^x p_i |\varphi_i^A\rangle \otimes |\phi_i^B\rangle, \quad (2.3)$$

where $\chi \leq \min(n_A, n_B)$ is the so-called Schmidt number and $p_i, i = 1, \dots, \chi$ are real, positive, and called the Schmidt coefficients. The coefficients are not unique but are always such that $\sum_{i=1}^{\chi} p_i^2 = 1$. If there exists a $i = 1, \dots, \chi$ such that $p_i = 1$, the state is in a product state, $|\psi\rangle = |\varphi_i^A\rangle \otimes |\phi_i^B\rangle$. By definition, it is therefore not entangled. Conversely, if we have at least two non-zero coefficients, the state is entangled. We refer to the Appendix A.1 of this thesis for a derivation of the Schmidt decomposition.

A key quantity to study the properties of a physical system is the density matrix [14]. The density matrix for the whole system is defined as

$$\rho = |\psi\rangle\langle\psi|. \quad (2.4)$$

The reduced density matrix of the subsystem A is obtained by taking the partial trace of ρ ,

$$\rho_A = \text{Tr}_{\mathcal{H}_B}(\rho) = \sum_{i=1}^{\chi} p_i^2 |\varphi_i^A\rangle\langle\varphi_i^A|, \quad (2.5)$$

where $\text{Tr}_{\mathcal{H}_B}$ denotes the partial trace over $\mathcal{H}_B$. The expression for the reduced density matrix of the subsystem B is analogous. Density matrices are Hermitian, $\rho^\dagger = \rho$, and such that

$$\text{Tr}_{\mathcal{H}}(\rho) = \text{Tr}_{\mathcal{H}_A}(\rho_A) = 1. \quad (2.6)$$

From the normalisation of $|\psi\rangle$, we have $\rho^2 = \rho$. Hence,

$$\text{Tr}(\rho^2) = 1. \quad (2.7)$$

We also use density matrices to compute the expectation values of operators. Let $\mathcal{O}$ be an operator acting on $\mathcal{H}$. Its expectation value in the state $|\psi\rangle$ is then given by

$$\langle\mathcal{O}\rangle = \langle\psi|\mathcal{O}|\psi\rangle = \text{Tr}(\rho\mathcal{O}). \quad (2.8)$$

We find a similar relation for an operator $\mathcal{O}_A$ acting in $\mathcal{H}_A$

$$\langle\mathcal{O}_A\rangle = \text{Tr}_{\mathcal{H}_A}(\rho_A\mathcal{O}_A). \quad (2.9)$$

Moreover, we recall that the logarithm of a matrix M is defined as

$$\log M = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} (M - \mathbb{I})^n. \quad (2.10)$$

To study the entanglement between the two subsystems, we use the so-called entanglement entropy [14]. The entropy for the subsystem A is defined as

$$S_A = S(\rho_A) = -\text{Tr}_{\mathcal{H}_A}(\rho_A \log \rho_A). \quad (2.11)$$

The entanglement entropy quantifies the entanglement in the following way. If A and B are not entangled, they are both in a pure state, and the entropy vanishes. If they are entangled, the entropy is a positive number and grows with the entanglement. As the subsystems are not pure states, there is a statistical uncertainty about the description of the systems. The entropy thus measures the amount of missing

information we have about one of the subsystems.

From (2.5), we see that the entropy can also be expressed as

$$S_A = - \sum_i p_i^2 \log p_i^2, \quad (2.12)$$

with the convention $0 \log 0 = 0$. Throughout the following, $\log$ always denotes the natural logarithm. Moreover, from the Schmidt decomposition, the coefficients p_i in the definition of ρ_A and ρ_B coincide. Thus, the entropies of both subsystems are equal: $S_A = S_B$.

Let us now consider a density matrix written as a tensor product: $\rho = \rho_A \otimes \rho_B$. The entropy satisfies an additive property [14]

$$S(\rho_A \otimes \rho_B) = S(\rho_A) + S(\rho_B). \quad (2.13)$$

We refer to the Appendix A.2 of this thesis for a proof of this property. By induction, the additivity is satisfied for a tensor product of n density matrices

$$S(\rho_1 \otimes \cdots \otimes \rho_n) = \sum_{i=1}^n S(\rho_i). \quad (2.14)$$

2.2 Bipartite fidelity

The second quantity we investigate is the so-called bipartite fidelity, which was introduced in 2011 by Stéphan and Dubail [12]. Before defining the bipartite fidelity, we introduce the concept of a quantum quench [15].

We consider a quantum system described by a Hamiltonian $\hat{H}$ that depends on a physical parameter λ . This parameter could, for instance, be an external magnetic field or the intensity of a laser. The system is prepared in its ground state with λ . At time $t = 0^+$, the parameter suddenly changes to $\lambda' \neq \lambda$. This process is called a quantum quench.

The bipartite fidelity is defined using a specific quantum quench [15]. We consider a bipartite quantum system described by the Hamiltonian

$$\hat{H} = \hat{H}_A + \hat{H}_B + \lambda \hat{H}^{\text{int}}, \quad (2.15)$$

where $\hat{H}_A$ and $\hat{H}_B$ are the Hamiltonians of the subsystems A and B , respectively, and are such that $[\hat{H}_A, \hat{H}_B] = 0$. The term $\hat{H}^{\text{int}}$ encompasses all the interactions between the subsystems, and λ is a parameter. The quantum quench considered for the bipartite fidelity is the change from $\lambda = 0$ to $\lambda = 1$.

Let us first consider $\lambda = 0$. The interactions between A and B are switched off and the system is composed of two independent subsystems. We denote this case by $A \otimes B$. Let $|A\rangle$ and $|B\rangle$ be the normalised ground states of $\hat{H}_A$ and $\hat{H}_B$, respectively. Since the subsystems are independent, there is no entanglement between

A and B . The ground state of $A \otimes B$ is then in a factorised state, $|A \otimes B\rangle = |A\rangle \otimes |B\rangle$.

After the quench, we have $\lambda = 1$. Thus, there are now interactions between the subsystems. These interactions produce entanglement between A and B . We denote this case by $A \cup B$ and its ground state by the normalised state $|A \cup B\rangle$. An example of such a situation is represented in Figure 2.1.

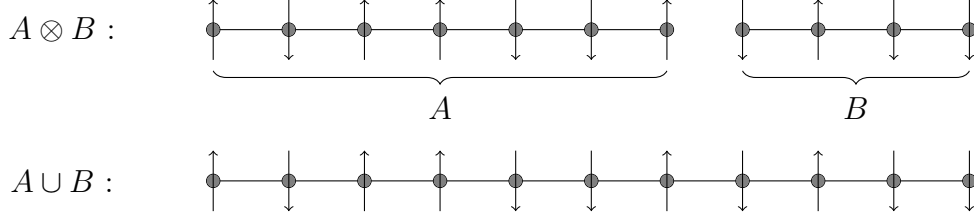


Figure 2.1: Example of a bipartition in the context of a one-dimensional spin system.

The bipartite fidelity is defined as the scalar product of the two ground states

$$\mathcal{B} = |\langle A \otimes B | A \cup B \rangle|^2. \quad (2.16)$$

It is interpreted as the probability of being in the ground state $|A \cup B\rangle$ after the quench. We also define the logarithmic bipartite fidelity (LBF) as

$$\mathcal{F} = -\log |\langle A \otimes B | A \cup B \rangle|^2. \quad (2.17)$$

The logarithmic bipartite fidelity is a measure of the similarity of the two ground states, $|A \cup B\rangle$ and $|A \otimes B\rangle$. It measures the entanglement between A and B in the following way. If after the quench, there is no interaction between the subsystems, the ground state $|A \cup B\rangle$ is in a product state and is equal to $|A \otimes B\rangle$, up to a phase. In this case, the bipartite of the two ground states is equal to one, and the LBF vanishes. Conversely, if the ground state $|A \cup B\rangle$ is not a product state, the two subsystems are entangled. As the ground state $|A \cup B\rangle$ differs from the factorised state, the overlap (2.16) decreases, and thus, the LBF increases.

One-dimensional quantum systems

For one-dimensional quantum critical systems,¹ Stéphan and Dubail predicted the leading and subleading terms of the bipartite fidelity using techniques from conformal field theory (CFT) [17]. The aim of our work is not to study the entanglement from a CFT point of view. It is, however, useful to borrow some known results from this field to later compare them with our results.

We consider a one-dimensional system of length N . The lengths of the subsystems A and B are N_A and N_B , respectively, and are such that $N = N_A + N_B$.

¹The notion of criticality in a quantum system depends on the spectrum of the Hamiltonian. In a critical model, the gap between the energy of the ground state and the energy of any excited level decreases as the inverse of the system's size. Such models are said to be gapless [16].

We denote the so-called central charge of the model by c and the so-called conformal weights by h_i , $i = 1, 2, 3, 4$. The weight h_2 is associated with the boundary-changing operator between the subsystems A and B . The other weights are associated with the ground state of subsystem A (h_1), subsystem B (h_3), and the whole system (h_4). Moreover, we define $\alpha_i = \pm\sqrt{2h_i}$. The association of the coefficients α_i to their respective systems is shown in Figure 2.2. In the case of a theory with $c = 1$, we have the relation $\sum_{i=1}^4 \alpha_i = 0$.

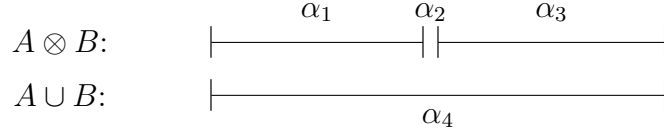


Figure 2.2: Representation of the coefficients α_i , $i = 1, \dots, 4$ and their associated systems.

Let us introduce the so-called aspect ratio $x = N_A/N$. The asymptotic expansion of the LBF for large N and fixed $x \in (0, 1)$ is given by [17]

$$\mathcal{F}(x) = \left(\frac{c}{8} + h_2\right) \log N + f(x) + g(x) \frac{\log N}{N} + \mathcal{O}\left(\frac{1}{N}\right), \quad (2.18)$$

with

$$\begin{aligned} f(x) &= \left[\frac{1}{24} \left(2x - 1 + \frac{2}{x} \right) + \left(1 - \frac{1}{x} \right) \alpha_1^2 - \frac{\alpha_2^2}{2} - \alpha_3^2 + (1-x)\alpha_4^2 \right] \log(1-x) \\ &\quad + \{x \rightarrow 1-x, \alpha_1 \leftrightarrow \alpha_3\} + \xi_f, \\ g(x) &= \xi_g \times \left[h_4 - \frac{1}{24} + \left(\frac{1}{24} - h_1 \right) \frac{1}{x} + \left(\frac{1}{24} - h_3 \right) \frac{1}{1-x} \right], \end{aligned} \quad (2.19)$$

where ξ_f, ξ_g are respectively an additive and a multiplicative constant which depend on the model considered.

The conformal weights h_i , $i = 1, 3, 4$, are related to the finite-size scaling of the ground state energy of their respective associated systems. For large L , the energy has the following expansion [18]:

$$E_0(L) = E_{\text{bulk}}L + E_{\text{bdry}} - \frac{\pi v_f}{24L} [c - 24h_i] + \mathcal{O}\left(\frac{1}{L^2}\right), \quad (2.20)$$

where $L = N, N_A, N_B$. The constants $E_{\text{bulk}}, E_{\text{bdry}}$ are non-universal and depend on the Hamiltonian considered. The factor v_F is the so-called Fermi velocity and can be accessed through Bethe ansatz techniques [19].

Comparison with the entanglement entropy

The logarithmic bipartite fidelity and the entanglement entropy share some similarities. Indeed, for instance, both quantities can be used to detect quantum phase

transitions [15]. They are both used to study entanglement, but their interpretation is different. The entanglement entropy is considered as an entanglement measure in a quantum information way [7] and measures the amount of missing information in a part of a composite system. This is not the case for the bipartite fidelity, which quantifies the similarity of the ground states before and after a quench. Moreover, the leading term of entropy in the ground state of one-dimensional critical models has a behaviour similar to the LBF. Indeed, in the scaling limit, Vidal et al. found that the entropy diverges as the logarithm of the subsystem's size [9]. However, there is no proportionality relation between the entanglement entropy and the bipartite fidelity.

Chapter 3

Free-fermion models and orthogonal polynomials

This chapter is dedicated to the introduction of spin chains. They are theoretical models used in condensed matter physics to investigate the behaviour of one-dimensional systems of interacting particles. They are particularly useful for understanding quantum magnetism [20], phase transitions, and critical phenomena [9, 21, 22, 23]. We are here interested in special cases of spin chains called free-fermions models with inhomogeneous interactions. These models are of particular interest as it is possible to diagonalise their Hamiltonian and explicitly construct its eigenstates. Moreover, it is possible to establish a link between free-fermion models and discrete orthogonal polynomials. That relation allows us to construct models based on families of polynomials.

3.1 Free-fermion model

We consider a system of $N \geq 0$ interacting particles with spin $1/2$ on a one-dimensional lattice that we call a chain. Each particle is localised on a site $j = 0, \dots, N - 1$ of the chain. We suppose that each particle only interacts with its nearest neighbours. The space of states of a single spin is $\mathbb{C}^2$. We denote its canonical basis by

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (3.1)$$

The space of states for the N spins is the tensor product $\mathcal{H} = (\mathbb{C}^2)^{\otimes N}$ of dimension 2^N . The spin operators acting on $\mathbb{C}^2$ are given by the usual Pauli matrices

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (3.2)$$

Furthermore, we define the spin operator of the spin $j = 0, \dots, N - 1$ of the chain as

$$\sigma_j^a = \mathbb{I} \otimes \cdots \otimes \mathbb{I} \otimes \underbrace{\sigma^a}_{j^{\text{th}}} \otimes \mathbb{I} \otimes \cdots \otimes \mathbb{I}, \quad a = x, y, z, \quad (3.3)$$

where $\mathbb{I}$ denotes the 2×2 identity matrix.

We consider systems with an external magnetic field B_n aligned in the z direction. The Hamiltonian for the chain of N spins with open boundary conditions is given by [24]

$$\hat{H} = \frac{1}{2} \sum_{n=0}^{N-2} J_n^x \sigma_n^x \sigma_{n+1}^x + J_n^y \sigma_n^y \sigma_{n+1}^y + J_n^z \sigma_n^z \sigma_{n+1}^z - \frac{1}{2} \sum_{n=0}^{N-1} B_n \sigma_n^z. \quad (3.4)$$

The real parameters $J_n^{x,y,z}$ are coupling constants and quantify the interactions between the spins. They depend on the direction of the spin projection x, y, z and thus allow anisotropy in the spin interactions.

The models we study are a special case of (3.4) with $J_n^x = J_n^y = J_n \neq 0$ and $J_n^z = 0$ for all $n = 0, \dots, N$. The Hamiltonian of the chain of N spins with open boundary conditions is thus given by

$$\hat{H} = \frac{1}{2} \sum_{n=0}^{N-2} J_n (\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y) - \frac{1}{2} \sum_{n=0}^{N-1} B_n \sigma_n^z. \quad (3.5)$$

To achieve periodic boundary conditions, we add

$$\frac{1}{2} J_{N-1} (\sigma_{N-1}^x \sigma_N^x + \sigma_{N-1}^y \sigma_N^y), \quad (3.6)$$

to the Hamiltonian and identify $\sigma_N^a = \sigma_0^a$, $a = x, y, z$. The different boundary conditions are represented in Figure 3.1.

We say that the model is inhomogeneous when the coupling constants J_n depend on n . Physically, it means that the interactions between the spins differ depending on where they are localised in the chain. Conversely, we say that a model is homogeneous if the coupling constants are independent of n . We refer to models described by the Hamiltonian (3.5) as free-fermion models. The motivation for this name will be clear later.

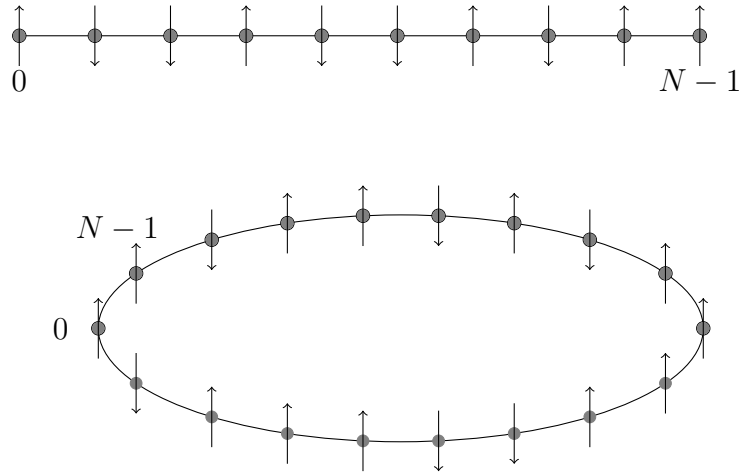


Figure 3.1: Representation of a spin chain with open boundary conditions (top) and with periodic boundary conditions (bottom).

3.1.1 Diagonalisation

To study the physical properties of the system, one must determine the spectrum of the Hamiltonian. In physics, we refer to the eigenvalues of the Hamiltonian as the energy levels and the eigenvectors as the eigenstates. This section is dedicated to the diagonalisation of the free-fermion Hamiltonian (3.5). The techniques we use here were first introduced by Lieb, Schultz, and Mattis for solving the XY chain [25]. This model is homogeneous and defined with $J^x, J^y \neq 0$ and $J^z = 0$. Hence, the models we consider are a special case of the XY chain with $J^x = J^y$. As the couplings are the same in the x and y directions, these models are usually called XX chains.

The first step is to perform the so-called Jordan-Wigner transform [26]. It maps a system of interacting spins onto an equivalent system of non-interacting (= free) spinless fermions. We first define the lowering and raising spin operators as

$$\sigma^\pm = \frac{\sigma^x \pm i\sigma^y}{2}. \quad (3.7)$$

Their action on a single spin up or down is

$$\begin{aligned} \sigma^+|\downarrow\rangle &= |\uparrow\rangle, & \sigma^+|\uparrow\rangle &= 0, \\ \sigma^-|\downarrow\rangle &= 0, & \sigma^-|\uparrow\rangle &= |\downarrow\rangle. \end{aligned} \quad (3.8)$$

The Jordan-Wigner transform is defined by the operators

$$c_j = (-1)^j \left(\prod_{n=0}^{j-1} \sigma_n^z \right) \sigma_j^-, \quad c_j^\dagger = (-1)^j \left(\prod_{n=0}^{j-1} \sigma_n^z \right) \sigma_j^+. \quad (3.9)$$

They satisfy the canonical anti-commutation relations for fermions:

$$\{c_j, c_i\} = \{c_j^\dagger, c_i^\dagger\} = 0, \quad \{c_i, c_j^\dagger\} = \delta_{ij}. \quad (3.10)$$

For that reason, we refer to such operators as fermionic operators. The Hamiltonian (3.5) written in terms of these fermionic operators is

$$\begin{aligned} \hat{H} &= \sum_{n=0}^{N-2} J_n (c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) - \sum_{n=0}^{N-1} B_n c_n^\dagger c_n \\ &= \sum_{n,m=0}^{N-1} H_{mn} c_m^\dagger c_n, \end{aligned} \quad (3.11)$$

where the matrix $H = (H_{mn})_{m,n=0}^{N-1}$ is

$$H = \begin{pmatrix} -B_0 & J_0 & 0 & \dots & 0 \\ J_0 & -B_1 & J_1 & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & J_{N-3} & -B_{N-2} & J_{N-2} \\ 0 & \dots & 0 & J_{N-2} & -B_{N-1} \end{pmatrix}. \quad (3.12)$$

To diagonalise the Hamiltonian, we first diagonalise the matrix H . We denote the

canonical basis of $\mathbb{C}^N$ by $\{|n\rangle, n = 0, \dots, N-1\}$. It is common in physics to refer to it as the position basis. In this basis, the matrix H is tridiagonal,

$$H|n\rangle = J_n|n+1\rangle - B_n|n\rangle + J_{n-1}|n-1\rangle, \quad k = 0, \dots, N-1, \quad (3.13)$$

with $J_{-1} = J_{N-1} = 0$. The matrix H is real and symmetric. By means of the spectral theorem [27], the matrix is diagonalisable by an orthogonal matrix. We denote the eigenvectors of H by $|\phi_k\rangle$. They satisfy the equation

$$H|\phi_k\rangle = \omega_k|\phi_k\rangle, \quad k = 0, \dots, N-1, \quad (3.14)$$

where ω_k is the eigenvalue associated with the eigenvector

$$|\phi_k\rangle = \sum_{n=0}^{N-1} \phi_{n,k}|n\rangle. \quad (3.15)$$

We choose the eigenvectors $|\phi_k\rangle$ real and such that they form an orthonormal basis of $\mathbb{C}^N$. We call this basis the momentum basis. The eigenfunctions $\phi_{n,k} = \langle n|\phi_k\rangle$ are real and satisfy the orthonormality condition

$$\sum_{n=0}^{N-1} \phi_{n,k}\phi_{n,p} = \delta_{kp}. \quad (3.16)$$

From (3.13), we find that the eigenfunctions satisfy a recurrence relation

$$\omega_k\phi_{n,k} = J_n\phi_{n+1,k} - B_n\phi_{n,k} + J_{n-1}\phi_{n-1,k}. \quad (3.17)$$

If $J_n \neq 0$ for all $n = 0, \dots, N-2$, each eigenfunction $\phi_{n+1,k}$ is entirely determined by $\phi_{n,k}$ and $\phi_{n-1,k}$. In particular, if we have $\phi_{0,k} = 0$, it follows that $\phi_{n,k} = 0$ for all $n = 1, \dots, N-1$. Hence, to ensure that $|\phi_k\rangle$ is non-zero, we must have $\phi_{0,k} \neq 0$.

Let us now suppose that there exist two eigenvectors, $|\phi_k\rangle$ and $|\phi_{k'}\rangle$, associated with the same eigenvalue ω_k . From the previous paragraph, we know that the first entry of both eigenvectors, $\phi_{0,k}$ and $\phi_{0,k'}$, is non-zero. By scaling, we can choose them such that $\phi_{0,k} = \phi_{0,k'} = 1$. Moreover, the difference $|\phi_k\rangle - |\phi_{k'}\rangle$ is also an eigenvector of H with eigenvalue ω_k and its first entry is zero. It follows that $|\phi_k\rangle - |\phi_{k'}\rangle$ is identically zero, and thus, $|\phi_k\rangle = |\phi_{k'}\rangle$. Hence, the eigenvalues of H are simple. We choose to order them such that

$$\omega_0 < \omega_1 < \dots < \omega_{N-1}. \quad (3.18)$$

From the orthonormality relation (3.16) and the realness of the eigenfunctions, the matrix elements of H are given by

$$H_{mn} = \langle m|H|n\rangle = \sum_{k=0}^{N-1} \omega_k \phi_{m,k} \phi_{n,k}. \quad (3.19)$$

Using this expression in (3.11), the Hamiltonian is now written as

$$\hat{H} = \sum_{k=0}^{N-1} \omega_k d_k^\dagger d_k, \quad d_k = \sum_{n=0}^{N-1} \phi_{n,k} c_n. \quad (3.20)$$

The operators $d_k, d_k^\dagger$, $k = 0, \dots, N-1$, are also fermionic operators as they obey the canonical anti-commutation relations for fermions. Indeed, from the anti-commutation relations of the operators $c_j, c_j^\dagger$, $j = 0, \dots, N-1$, and the orthonormality relation (3.16), we have

$$\begin{aligned} \{d_k^\dagger, d_k\} &= \sum_{i,j=0}^{N-1} \phi_{i,k} \phi_{j,l} \{c_i^\dagger, c_j\} = \sum_{i=0}^{N-1} \phi_{i,k} \phi_{i,l} = \delta_{kl}, \\ \{d_k, d_l\} &= \sum_{i,j=0}^{N-1} \phi_{i,k} \phi_{j,l} \{c_i, c_j\} = 0, \quad \{d_k^\dagger, d_l^\dagger\} = \sum_{i,j=0}^{N-1} \phi_{i,k} \phi_{j,l} \{c_i^\dagger, c_j^\dagger\} = 0. \end{aligned} \quad (3.21)$$

3.1.2 Eigenstates

In this section, we explicitly construct the eigenstates of the Hamiltonian $\hat{H}$. Let us first define the so-called fermion number operator as

$$F = \sum_{k=0}^{N-1} d_k^\dagger d_k = \sum_{j=0}^{N-1} c_j^\dagger c_j. \quad (3.22)$$

As the name suggests, it counts the number of fermions in a given state $|\psi\rangle$:

$$F|\psi\rangle = \eta|\psi\rangle, \quad (3.23)$$

where η is an eigenvalue of F and the number of fermions in $|\psi\rangle$. From its definition, we see that the fermion number operator commutes with the Hamiltonian (3.20), $[F, \hat{H}] = 0$. Therefore, they share the same eigenvectors.

Let us now introduce the vacuum state of the system $|0\rangle$ as the state with zero fermion. In view of the Jordan-Wigner transformation, it corresponds to the state where all the spins are down: $|0\rangle = |\downarrow \dots \downarrow\rangle$. The vacuum state satisfies

$$c_j|0\rangle = 0, \quad j = 0, \dots, N-1, \quad (3.24)$$

or, equivalently,

$$d_k|0\rangle = 0, \quad k = 0, \dots, N-1. \quad (3.25)$$

We assume that the vacuum state is a normalised state: $\langle 0|0\rangle = 1$. It is an eigenvector of F with eigenvalue 0. We now investigate the action of $d_k^\dagger$ on an eigenvector of F . We denote $|\psi'\rangle = d_k^\dagger|\psi\rangle$. To count the number of fermions in $|\psi'\rangle$, we act with F on it:

$$F|\psi'\rangle = Fd_k^\dagger|\psi\rangle = ([F, d_k^\dagger] + d_k^\dagger F)|\psi\rangle. \quad (3.26)$$

The commutator is given by $[F, d_k^\dagger] = d_k^\dagger$. Thus, we have

$$\begin{aligned} F|\psi'\rangle &= (d_k^\dagger + d_k^\dagger F)|\psi\rangle \\ &= d_k^\dagger (F + \mathbb{I})|\psi\rangle \\ &= d_k^\dagger (\eta + 1)|\psi\rangle = (\eta + 1)|\psi'\rangle. \end{aligned} \quad (3.27)$$

Hence, the action of $d_k^\dagger$ on an eigenvector of F with η fermions yields an eigenvector with $\eta + 1$ fermions. For that reason, the operator $d_k^\dagger$ is called a creation operator. Conversely, the operator d_k is an annihilation operator as its action on an eigenvector of F yields a state with one less fermion.

As $d_k|0\rangle = 0$, we cannot have a state with a negative number of fermions. Moreover, by means of Pauli's principle [28], two or more fermions cannot simultaneously occupy the same quantum state. Hence, we cannot have more than N fermions in our system. The eigenvalues of F are thus $\eta \in \{0, \dots, N\}$.

The eigenstates of the Hamiltonian $\hat{H}$ are then constructed by acting with the fermion creation operator $d_k^\dagger$ on the vacuum state:

$$|\psi\rangle = \prod_{i=0}^{\eta} d_{k_i}^\dagger |0\rangle, \quad k_1 \neq \dots \neq k_\eta \in \{0, \dots, N-1\}. \quad (3.28)$$

From the normalisation of the vacuum state and the action of the $d_k, d_k^\dagger$ operators, the eigenstates (3.28) are normalised. They satisfy the relation

$$H|\psi\rangle = E|\psi\rangle, \quad E = \sum_{i=1}^{\eta} \omega_{k_i}, \quad (3.29)$$

where E is the energy level of the state $|\psi\rangle$. In particular, the vacuum state is a state with zero energy.

Ground state

Let us now focus on the ground state of the system, that is, the state with the lowest energy level. To this end, we must choose $k_1, \dots, k_\eta$ such that E is minimal.

Recall that we have ordered $\omega_0 < \omega_1 < \dots < \omega_{N-1}$. If the eigenvalues are all non-negative, the ground state corresponds to the vacuum state. If some eigenvalues are negative, the lowest energy level is achieved if we consider the k_i 's such that the ω_{k_i} are negative. We define f an integer such that $\omega_{f-1} \leq 0$ and $\omega_f > 0$. Thus, the ground state is a state filled with f fermions defined as

$$|\psi_0\rangle = \prod_{k=0}^{f-1} d_k^\dagger |0\rangle, \quad (3.30)$$

and its energy is

$$E_0 = \sum_{k=0}^{f-1} \omega_k. \quad (3.31)$$

We note that the eigenvalues ω_k can be shifted, and thus the value of f modified, by adding a constant term to the magnetic field B_n in the Hamiltonian (3.11). This change does not affect the eigenstates.

3.2 Entanglement entropy in spin chains

To compute the entanglement entropy in a bipartite system, one has to find the eigenvalues of the reduced density matrix of one of the subsystems (2.11). For free-fermion models, it is possible to relate the eigenvalues of the reduced density matrix to the eigenvalues of the so-called reduced correlation matrix, which is the matrix of the two-point functions of the system [29]. In this section, we follow [13, 30] to derive a closed form of the entropy based on that relation.

From now on, we study the ground state of the system, unless otherwise indicated. We write the expectation value of an operator $\mathcal{O}$ in the ground state as $\langle \mathcal{O} \rangle = \langle \psi_0 | \mathcal{O} | \psi_0 \rangle$. We define the correlation matrix of the system as the matrix of the two-point functions

$$\hat{C} = (\langle c_m^\dagger c_n \rangle)_{m,n=0}^{N-1}. \quad (3.32)$$

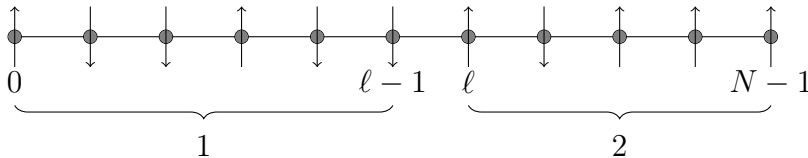
To evaluate the matrix elements, we first look at the two-point function of the d_k and $d_k^\dagger$ operators. From the definition of the ground state (3.30), we deduce that it is annihilated by the $d_k^\dagger$ operators when $\omega_k \leq 0$ (i.e., $d_k^\dagger |\psi_0\rangle = 0$) and by the d_k operators when $\omega_k > 0$ (i.e., $d_k |\psi_0\rangle = 0$). Therefore, we find

$$\langle d_k^\dagger d_l \rangle = \begin{cases} \delta_{kl}, & \text{for } k = 0, \dots, f-1, \\ 0, & \text{otherwise.} \end{cases} \quad (3.33)$$

Using the transform (3.20), we find that the two-point function of the $c_j, c_j^\dagger$ operators is given by

$$\hat{C}_{mn} = \langle c_m^\dagger c_n \rangle = \sum_{k,l=0}^{N-1} \phi_{m,k} \phi_{n,l} \langle d_k^\dagger d_l \rangle = \sum_{k=0}^{f-1} \phi_{m,k} \phi_{n,k}, \quad m, n = 0, \dots, N-1. \quad (3.34)$$

We aim to compute the entanglement entropy between two subsystems of our chain of N sites in the ground state. We define the first subsystem as the collection of spins localised on the first ℓ sites, and the second one as the collection of spins localised in the rest of the chain.



We define the reduced correlation matrix of the first subsystem C as the $\ell \times \ell$ submatrix of $\hat{C}$, $C = (\hat{C}_{mn})_{0 \leq m,n \leq \ell-1}$. The reduced correlation matrix C is a real and symmetric matrix. Hence, it is diagonalisable by a unitary matrix $U = (u_{mn})_{m,n=0}^{\ell-1}$,

$$\sum_{m,n=0}^{\ell-1} u_{mp}^* C_{mn} u_{nq} = \nu_p \delta_{pq}, \quad (3.35)$$

where ν_m denotes the eigenvalues of C . We define a new set of operators in this basis

$$g_p = \sum_{n=0}^{\ell-1} u_{np} c_n, \quad g_p^\dagger = \sum_{n=0}^{\ell-1} u_{np}^* c_n^\dagger. \quad (3.36)$$

From the unitarity of U and the anti-commutation relations of the operators $c_n, c_n^\dagger$, the operators (3.36) are also fermionic operators

$$\begin{aligned} \{g_p, g_p^\dagger\} &= \sum_{m,n=0}^{\ell-1} u_{mp} u_{nq}^* \{c_m, c_n^\dagger\} = \sum_{n=0}^{\ell-1} u_{np}^* u_{nq} = (U^\dagger U)_{pq} = \delta_{pq}, \\ \{g_p, g_q\} &= \sum_{m,n=0}^{\ell-1} u_{mp} u_{nq} \{c_n, c_m\} = 0, \quad \{g_p^\dagger, g_q^\dagger\} = \sum_{m,n=0}^{\ell-1} u_{mp}^* u_{nq}^* \{c_n^\dagger, c_m^\dagger\} = 0. \end{aligned} \quad (3.37)$$

Using the transform (3.36) in (3.35), it follows that

$$\langle g_p^\dagger g_q \rangle = \nu_p \delta_{pq}, \quad (3.38)$$

for $p, q = 0, \dots, \ell - 1$. The operators $g_p, g_p^\dagger$ define a new system of ℓ fermions in a chosen basis. We denote the Hilbert space of the system by $\mathcal{H}_\ell$. The operators $g_p, g_p^\dagger$ are creation and annihilation operators for fermions in that system. In their computational basis, they thus have the matrix representation

$$g = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad g^\dagger = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \quad (3.39)$$

Let us now define the operators [30]

$$\mathcal{O}_p^0 = g_p^\dagger g_p, \quad \mathcal{O}_p^1 = g_p g_p^\dagger, \quad \mathcal{O}_p^2 = g_p, \quad \mathcal{O}_p^3 = g_p^\dagger, \quad (3.40)$$

with $p = 0, \dots, \ell - 1$. The set of operators $\left\{ \prod_{i=0}^{\ell-1} \mathcal{O}_i^{\varepsilon_i}, \varepsilon_i = 0, 1, 2, 3 \right\}$ forms an orthonormal basis for the operator acting on $\mathcal{H}_\ell$ [30]. It is thus possible to write the density matrix in terms of that product of operators as

$$\rho_\ell = \sum_{0 \leq \varepsilon_0, \dots, \varepsilon_{\ell-1} \leq \ell-1} \Xi^{\varepsilon_0, \dots, \varepsilon_{\ell-1}} \prod_{i=0}^{\ell-1} \mathcal{O}_i^{\varepsilon_i}, \quad (3.41)$$

with

$$\Xi^{\varepsilon_0, \dots, \varepsilon_{\ell-1}} = \text{Tr}_{\mathcal{H}_\ell} \left((\mathcal{O}_0^{\varepsilon_0} \dots \mathcal{O}_{\ell-1}^{\varepsilon_{\ell-1}})^\dagger \rho_\ell \right) = \langle (\mathcal{O}_0^{\varepsilon_0} \dots \mathcal{O}_{\ell-1}^{\varepsilon_{\ell-1}})^\dagger \rangle. \quad (3.42)$$

By means of Wick's theorem [28], we can write $\Xi^{\varepsilon_0, \dots, \varepsilon_{\ell-1}}$ in terms of the two-point functions of the operators $g_p, g_p^\dagger$. Moreover, we find that

$$\langle g_p g_q \rangle = \langle g_p^\dagger g_q^\dagger \rangle = 0, \quad \langle g_p^\dagger g_q \rangle = \nu_p \delta_{pq}, \quad \langle g_p g_q^\dagger \rangle = (1 - \nu_p) \delta_{pq}. \quad (3.43)$$

Therefore, the only elements that do not vanish in (3.42) are those with $\varepsilon_i = 0, 1$, $i = 0, \dots, \ell - 1$. Thus, we write (3.42) as

$$\Xi^{\varepsilon_0, \dots, \varepsilon_{\ell-1}} = \prod_{i=0}^{\ell-1} \langle \mathcal{O}_i^{\varepsilon_i} \rangle, \quad \varepsilon_i = 0, 1. \quad (3.44)$$

The reduced density matrix (3.41) is then given by

$$\begin{aligned}\rho_\ell &= \prod_{i=0}^{\ell-1} \langle \mathcal{O}_i^0 \rangle \mathcal{O}_i^0 + \langle \mathcal{O}_i^1 \rangle \mathcal{O}_i^1 \\ &= \prod_{i=0}^{\ell-1} \nu_i g_i^\dagger g_i + (1 - \nu_i) g_i g_i^\dagger.\end{aligned}\tag{3.45}$$

It follows that the density matrix can be decomposed into a tensor product:

$$\rho_\ell = \varrho_0 \otimes \cdots \otimes \varrho_{\ell-1},\tag{3.46}$$

where $\varrho_i = \nu_i g^\dagger g + (1 - \nu_i) g g^\dagger$, $i = 0, \dots, \ell - 1$. From the definition of the von Neumann entropy (2.11) and the additive property (2.14), we find that the entropy of the block of ℓ spins is

$$S_\ell = \sum_{m=0}^{\ell-1} S(\varrho_m) = - \sum_{m=0}^{\ell-1} \nu_m \log(\nu_m) + (1 - \nu_m) \log(1 - \nu_m).\tag{3.47}$$

This formula allows us to compute the entropy only from the eigenvalues of the reduced density matrix.

3.2.1 Discussion

The formula (3.47) is particularly convenient for numerical analysis as it only requires the eigenvalues of C . However, Crampé et al. showed that it was also possible to find the eigenvalues without involving the direct diagonalisation of the reduced correlation matrix [31]. They investigated the existence of a tridiagonal matrix that commutes with the reduced correlation matrix. If such a matrix exists, it shares the same eigenvectors as the reduced correlation matrix. Hence, it would be possible to compute the eigenvalues of the reduced correlation matrix using the eigenvectors found directly from the tridiagonal commuting matrix.

The correlation matrix (3.34) can also be written as

$$\hat{C} = \sum_{k=0}^{f-1} |\phi_k\rangle \langle \phi_k|,\tag{3.48}$$

and the reduced correlation matrix as

$$C = \pi_1 \pi_2 \pi_1,\tag{3.49}$$

with

$$\pi_1 = \sum_{n=0}^{\ell-1} |n\rangle \langle n|, \quad \pi_2 = \hat{C} = \sum_{k=0}^{f-1} |\phi_k\rangle \langle \phi_k|.\tag{3.50}$$

Thus, finding a matrix T such that $[T, \pi_1] = [T, \pi_2] = 0$ is a sufficient condition for $[T, C] = 0$. We will see in Section 3.5 how to construct such a matrix.

3.3 Discrete orthogonal polynomials

We have seen that the eigenfunctions satisfy a three-term recurrence relation (3.17) and an orthonormality relation (3.16). It is therefore natural to think of relating them to orthogonal polynomials since it is well known that they satisfy similar relations. In this section, we briefly review some properties of discrete orthogonal polynomials [32, 33].

Let N be an integer and $X = \{0, \dots, N-1\}$ a finite set of $\mathbb{R}$. We consider a finite system of polynomials $\{P_n(x)\}_{n=0}^{N-1}$ on the real line with degree $[P_n(x)] = n$ for all $n = \{0, 1, \dots, N-1\}$. Let $w(x)$, $x \in X$, be a positive discrete weight function on X . We define a scalar product on the real vector space of polynomials by

$$\langle P_n, P_m \rangle = \sum_{x=0}^{N-1} w(x) P_n(x) P_m(x). \quad (3.51)$$

The system $\{P_n(x)\}_{n=0}^N$ is called orthogonal on X with respect to the weight $w(x)$ if

$$\sum_{x=0}^{N-1} w(x) P_n(x) P_m(x) = v_n \delta_{nm}, \quad w(x), v_n > 0, \quad (3.52)$$

for $m, n \in \{0, 1, \dots, N-1\}$ and v_n the square norm. We refer to such polynomials as discrete orthogonal polynomials. They satisfy similar relations as their continuous analogues.

Proposition 3.3.1. *The orthogonal polynomials P_n satisfy a three-term recurrence relation*

$$xP_n(x) = A_n P_{n+1}(x) + B_n P_n(x) + C_n P_{n-1}(x), \quad (3.53)$$

with $C_0 = A_{N-1} = 0$ and

$$\begin{aligned} A_n &= \frac{1}{v_{n+1}} \langle xP_{n+1}, P_n \rangle, \\ B_n &= \frac{1}{v_n} \langle xP_n, P_n \rangle, \\ C_n &= \frac{1}{v_{n-1}} \langle xP_{n-1}, P_n \rangle. \end{aligned} \quad (3.54)$$

Proof. The polynomial $xP_n(x)$ has a degree of $n+1$ and can be expanded in the basis of polynomials up to degree $n+1$ as [33]

$$xP_n(x) = \sum_{k=0}^{n+1} c_{k,n} P_k(x). \quad (3.55)$$

Taking the scalar product with P_m on both sides of the above equation, we find, for $m = 0, \dots, n+1$,

$$\langle P_m, xP_n \rangle = \sum_{k=0}^{n+1} c_{k,n} \langle P_m, P_k \rangle = c_{m,n} \langle P_m, P_m \rangle = c_{m,n} v_m. \quad (3.56)$$

We have $\langle P_m, xP_n \rangle = \langle xP_m, P_n \rangle$. By orthogonality, this scalar product is equal to zero when $m + 1 < n$. Since the square norm is non-zero, this implies that

$$c_{m,n} = 0, \quad \text{if } m = 0, \dots, n-1. \quad (3.57)$$

Thus, we only have three non-zero terms, and the expansion of $xP_n(x)$ is now

$$xP_n(x) = c_{n-1,n}P_{n-1}(x) + c_{n,n}P_n(x) + c_{n+1,n}P_{n+1}(x). \quad (3.58)$$

We identify $c_{n+1,n}, c_{n,n}, c_{n-1,n}$ with A_n, B_n, C_n , respectively, and the conclusion follows. $\square$

A direct consequence of the recurrence relation is the Christoffel-Darboux formula.

Proposition 3.3.2. *The orthogonal polynomials P_n satisfy the Christoffel-Darboux identity*

$$\sum_{j=0}^n \frac{P_j(x)P_j(y)}{v_j} = \begin{cases} \frac{A_n}{v_n} \frac{[P_{n+1}(x)P_n(y) - P_n(x)P_{n+1}(y)]}{x-y}, & \text{if } x \neq y, \\ \frac{A_n}{v_n} [P'_{n+1}(x)P_n(x) - P_{n+1}(x)P'_n(x)], & \text{if } x = y, \end{cases} \quad (3.59)$$

where A_n is the coefficient in the recurrence relation and v_n the square norm.

Proof. Let us first multiply the sum by x . Using the recurrence relation, we have

$$\begin{aligned} x \sum_{j=0}^n \frac{P_j(x)P_j(y)}{v_j} &= \sum_{j=0}^n \frac{xP_j(x)P_j(y)}{v_j} \\ &= \sum_{j=0}^n (A_jP_{j+1}(x) + B_jP_j(x) + C_jP_{j-1}(x)) \frac{P_j(y)}{v_j} \\ &= \frac{A_n}{v_n} P_{n+1}(x)P_n(y) + \sum_{j=0}^n \frac{B_j}{v_j} P_j(x)P_j(y) \\ &\quad + \sum_{j=0}^{n-1} \left(\frac{A_j}{v_j} P_{j+1}(x)P_j(y) + \frac{C_{j+1}}{v_{j+1}} P_j(x)P_{j+1}(y) \right). \end{aligned} \quad (3.60)$$

We find a similar result for $y \sum_{j=0}^n P_j(x)P_j(y)/v_j$. Therefore, for $x \neq y$, we have

$$\begin{aligned} (x-y) \sum_{j=0}^n \frac{P_j(x)P_j(y)}{v_j} &= \frac{A_n}{v_n} (P_{n+1}(x)P_n(y) - P_n(x)P_{n+1}(y)) \\ &\quad + \sum_{j=0}^{n-1} \left(\frac{A_j}{v_j} - \frac{C_{j+1}}{v_{j+1}} \right) (P_{j+1}(x)P_j(y) - P_j(x)P_{j+1}(y)). \end{aligned} \quad (3.61)$$

From the definition of the coefficients A_j and C_j (3.54), we see that $A_j v_{j+1} = C_{j+1} v_j$. Thus, the remaining sum cancels, and we find the case $x \neq y$ of (3.59). The result for $x = y$ is found by taking the limit $y \rightarrow x$ of the $x \neq y$ case. $\square$

Hypergeometric functions

We now introduce the hypergeometric function ${}_rF_s$ defined by the series [32]

$${}_rF_s \left(\begin{matrix} a_1, \dots, a_r \\ b_1, \dots, b_s \end{matrix}; z \right) = \sum_{k=0}^{\infty} \frac{(a_1)_k \cdots (a_r)_k}{(b_1)_k \cdots (b_s)_k} \frac{z^k}{k!}, \quad (3.62)$$

where $(a)_k$ is the Pochhammer symbol defined as, for $a > 0$,

$$(a)_k = \frac{\Gamma(a+k)}{\Gamma(a)} = \begin{cases} 1, & k = 0, \\ a(a+1) \cdots (a+k-1), & k = 1, 2, 3, \dots \end{cases} \quad (3.63)$$

We note the following identity involving the Pochhammer symbol, for k a non-negative integer and $a > 0$,

$$\binom{a}{k} = (-1)^k \frac{(-a)_k}{k!}. \quad (3.64)$$

We investigate in more detail the special case of the hypergeometric function for $r = 2$ and $s = 1$,

$${}_2F_1 \left(\begin{matrix} a, & b \\ & c \end{matrix}; z \right) = \sum_{k=0}^{\infty} \frac{(a)_k (b)_k}{(c)_k} \frac{z^k}{k!}. \quad (3.65)$$

The parameters must be such that the denominator is never zero in each term of the series. If either a or b are equal to $-n$, with n a non-negative integer, the series terminates at $k = n$ since $(-n)_k = 0$ for all $k > n$. Therefore, the series defines a polynomial in the variable z :

$${}_2F_1 \left(\begin{matrix} -n, & b \\ & c \end{matrix}; z \right) = \sum_{k=0}^n \frac{(-n)_k (b)_k}{(c)_k} \frac{z^k}{k!}. \quad (3.66)$$

If both $a = -n$ and $b = -m$, with n, m non-negative integers, the series terminates at $k = \min(n, m)$. Furthermore, if $c = -N$, N a non-negative integer, the series is well-defined if and only if at least one parameter in the numerator is also negative, $a = -n$ with $n \in \{0, \dots, N\}$. Indeed, for all $k' \in \{0, \dots, N\}$ such that $(-N)_{k'} = 0$, there exists k such that $k < k'$ and $(-a)_k = 0$.

3.4 Free-fermion models and orthogonal polynomials

In Section 3.1, we derived some properties of the eigenfunctions $\phi_{n,k}$ related to the eigenvalue problem of the matrix H (3.14). We then noticed that these properties were similar to the ones that discrete orthogonal polynomials satisfied. In this section, we follow [31] and construct free-fermion models based on orthogonal polynomials using these similarities.

We consider polynomials from the so-called Askey scheme [32]. The Askey scheme is a way of organising orthogonal polynomials of hypergeometric type into a hierarchy. The orthogonality relation for these polynomials is

$$\sum_{x=0}^{N-1} w(x) P_m(x) P_n(x) = v_n \delta_{nm}, \quad w(x), v_n > 0 \quad (3.67)$$

with $P_0(x) = 1$. Their three-term recurrence relation has the form

$$\lambda(x)P_n(x) = A_n P_{n+1}(x) - [A_n + C_n] P_n(x) + C_n P_{n-1}(x), \quad 0 \leq n \leq N-1, \quad (3.68)$$

with $C_0 = A_{N-1} = 0$. Note that we have written $\lambda(x)$ instead of x as it was the case in (3.53). Here, $\lambda(x)$ denotes a linear function of x . The motivation for this change is to later match some conventions or constraints of the physical models. The coefficients A_n , C_n are modified accordingly so the recurrence relation holds. Polynomials from the Askey scheme also satisfy a difference relation given by

$$f(n)P_n(x) = \bar{A}(x)P_n(x+1) - [\bar{A}(x) + \bar{C}(x)] P_n(x) + \bar{C}(x)P_n(x-1), \quad 0 \leq x \leq N-1, \quad (3.69)$$

with $\bar{C}(0) = \bar{A}(N-1) = 0$. The factor $f(n)$ is a linear function of n . The justification is analogous to the one for the factor $\lambda(x)$ in the recurrence relation.

We now establish a link between the eigenfunctions and the orthogonal polynomials. The recurrence relation for the eigenfunctions (3.17) can be mapped onto the one for the polynomials (3.68) if we consider polynomials of the form

$$P_n(x) = \frac{\alpha_n}{\sqrt{w_k}} \phi_{n,k}, \quad (3.70)$$

where α_n is a coefficient that will be determined for each set of orthogonal polynomials considered. We use this expression to compare the different relations of the polynomials and the eigenfunctions. From the recurrence relations (3.68) and (3.17), we identify

$$x = k, \quad \lambda(x) = \omega_k, \quad w_k = w(x), \quad J_n = \frac{\alpha_{n+1}}{\alpha_n} A_n = \frac{\alpha_n}{\alpha_{n+1}} C_{n+1}, \quad B_n = A_n + C_n. \quad (3.71)$$

We determine the α_n coefficient with, for $\epsilon = \pm 1$,

$$\begin{aligned} \alpha_n &= \pm \alpha_{n-1} \sqrt{\frac{C_n}{A_{n-1}}} \\ &= \epsilon \alpha_0 \prod_{i=1}^n \sqrt{\frac{C_i}{A_{i-1}}}. \end{aligned} \quad (3.72)$$

This expression is well-defined as the recurrence coefficient A_n is non-zero for all $n = 0, \dots, N-2$. The physical parameters are then given by

$$J_n = \epsilon \sqrt{C_{n+1} A_n}, \quad B_n = A_n + C_n \quad (3.73)$$

From the difference relation (3.69), we see that the eigenfunctions also obey a dual relation

$$\lambda_n \phi_{n,k} = \bar{J}_k \phi_{n,k+1} - \bar{B}_k \phi_{n,k} + \bar{J}_{k-1} \phi_{n,k-1}, \quad (3.74)$$

with

$$\lambda_n = f(n), \quad \bar{J}_k = \bar{A}(k) \sqrt{\frac{W_k}{W_{k+1}}} = \bar{C}(k+1) \sqrt{\frac{W_{k+1}}{W_k}}, \quad \bar{B}_k = \bar{A}(k) + \bar{C}(k). \quad (3.75)$$

3.5 Construction of a commuting matrix

We have already discussed in Section 3.2.1 how the existence of a matrix that commutes with the reduced correlation matrix would be useful in the investigation of the entropy. This section is dedicated to the construction of such a matrix, following [31].

Let us first define a new operator X which is diagonal in the position basis,

$$X|n\rangle = \lambda_n|n\rangle, \quad n = 0, \dots, N-1. \quad (3.76)$$

Using the difference relation for the eigenfunctions (3.74), we see that this operator is tridiagonal in the momentum basis,

$$X|\phi_k\rangle = \bar{J}_k|\phi_{k+1}\rangle - \bar{B}_k|\phi_k\rangle + \bar{J}_{k-1}|\phi_{k-1}\rangle. \quad (3.77)$$

The operators H and X are thus such that in one basis, H is tridiagonal and X is diagonal and in another basis, H is diagonal and X is tridiagonal. We now define the operator $\hat{T}$ as

$$\hat{T} = \{X, H\} + \tau_1[X, H] + \tau_2 X + \tau_3 H, \quad (3.78)$$

where τ_1, τ_2 and τ_3 are coefficients that we determine later. This operator is known as the algebraic Heun operator [34]. Notice that $\hat{T}$ is tridiagonal in both the position basis,

$$\begin{aligned} \hat{T}|n\rangle &= J_n(\lambda_{n+1}(1 + \tau_1) + \lambda_n(1 - \tau_1) + \tau_3)|n+1\rangle \\ &\quad + (\tau_2\lambda_n - B_n\tau_3 - 2B_n\lambda_n)|n\rangle \\ &\quad + J_{n-1}(\lambda_{n-1}(1 + \tau_1) + \lambda_n(1 - \tau_1) + \tau_3)|n-1\rangle, \end{aligned} \quad (3.79)$$

and the momentum basis,

$$\begin{aligned} \hat{T}|\phi_k\rangle &= \bar{J}_k(\omega_k(1 + \tau_1) + \omega_{k+1}(1 - \tau_1) + \tau_2)|\phi_{k+1}\rangle \\ &\quad + (\tau_3\omega_k - 2\bar{B}_k\omega_k - \tau_2\bar{B}_k)|\phi_k\rangle \\ &\quad + \bar{J}_{k-1}(\omega_k(1 + \tau_1) + \omega_{k-1}(1 - \tau_1) + \tau_2)|\phi_{k-1}\rangle. \end{aligned} \quad (3.80)$$

Let T denote the chopped matrix, $T = (\hat{T}_{mn})_{0 \leq m, n \leq \ell-1}$. We determine the parameters τ_1, τ_2, τ_3 such that $[T, \pi_1] = [T, \pi_2] = 0$, which is equivalent to

$$\begin{cases} T\pi_1|n\rangle = \pi_1 T|n\rangle, & \text{for all } n = 0, \dots, N-1, \\ T\pi_2|\phi_k\rangle = \pi_2 T|\phi_k\rangle, & \text{for all } k = 0, \dots, N-1. \end{cases} \quad (3.81)$$

Recall that π_1, π_2 are defined by (3.50). They are such that

$$\pi_1|n\rangle = \begin{cases} |n\rangle & \text{if } n \leq \ell-1, \\ 0 & \text{otherwise,} \end{cases} \quad (3.82)$$

and

$$\pi_2|\phi_k\rangle = \begin{cases} |\phi_k\rangle & \text{if } k \leq f-1, \\ 0 & \text{otherwise.} \end{cases} \quad (3.83)$$

To find the parameters τ_1, τ_2 and τ_3 , we evaluate the first relation in (3.81) at $n = \ell - 1, \ell$ and the second one at $k = f - 1, f$. We find that the commutation relations are satisfied when

$$\tau_1 = 0, \quad \tau_2 = -(\omega_{f-1} + \omega_f), \quad \tau_3 = -(\lambda_{\ell-1} + \lambda_\ell). \quad (3.84)$$

Thus, in the position basis, T is defined by a tridiagonal matrix

$$T = \begin{pmatrix} d_0 & t_0 & 0 & \dots & 0 \\ t_0 & d_1 & t_1 & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & t_{\ell-3} & d_{\ell-2} & t_{\ell-2} \\ 0 & \dots & 0 & t_{\ell-2} & d_{\ell-1} \end{pmatrix}. \quad (3.85)$$

with

$$\begin{cases} t_n &= J_n(\lambda_n + \lambda_{n+1} - \lambda_{\ell-1} - \lambda_\ell) \\ d_n &= -\lambda_n(\omega_{f-1} + \omega_f) - B_n(2\lambda_n - \lambda_{\ell-1} - \lambda_\ell). \end{cases} \quad (3.86)$$

From Section 3.2.1, this matrix, by construction, commutes with the reduced correlation matrix: $[T, C] = 0$. They thus share the same eigenvectors. Therefore, it is possible to act with C on the eigenvectors computed from T and then find the eigenvalues of C .

Chapter 4

XX spin chain

We have seen in the previous chapter how to construct free-fermion models based on orthogonal polynomials. We now apply this formalism to specific families of orthogonal polynomials. The first polynomials we consider are the Chebyshev polynomials of the second kind. They lead to a well-known model called the XX chain [31]. We study the entanglement entropy and the bipartite fidelity in the ground state and the first excited state of the model.

4.1 Chebyshev polynomials

The Chebyshev polynomials of the second kind of degree n are defined by

$$U_n(x) = \frac{\sin((n+1)\theta)}{\sin \theta}, \quad n = 0, 1, \dots, \quad (4.1)$$

with $x = \cos \theta$. Here, x is not restricted to integer values. They are part of the Askey scheme as they also have an expression in terms of a hypergeometric function [32]. For our investigations, however, it is not necessary to use the hypergeometric representation. The Chebyshev polynomials satisfy the recurrence relation

$$(2x - 2)U_n(x) = U_{n+1}(x) - 2U_n(x) + U_{n-1}(x). \quad (4.2)$$

with $U_0(x) = 1$ and $U_1(x) = 2x$. The graphs of the first few polynomials are represented in Figure 4.1.

4.2 The model

To construct the model, we make use of a certain discretisation of the continuous Chebyshev polynomials. The recurrence relation of the Chebyshev polynomials (4.2) has the form (3.68). Thus, we apply all the formalism of Section 3.4 to this specific family of polynomials. After multiplying both sides of (4.2) by -1 for convention, we find

$$\lambda(x) = -2x + 2, \quad A_0 = \dots = A_{N-2} = -1, \quad C_1 = \dots = C_{N-1} = -1. \quad (4.3)$$

From (3.73), we deduce that the physical parameters of the models are given by, choosing $\epsilon = -1$,

$$J_0 = \dots = J_{N-2} = -1, \quad B_0 = \dots = B_{N-1} = -2, \quad (4.4)$$

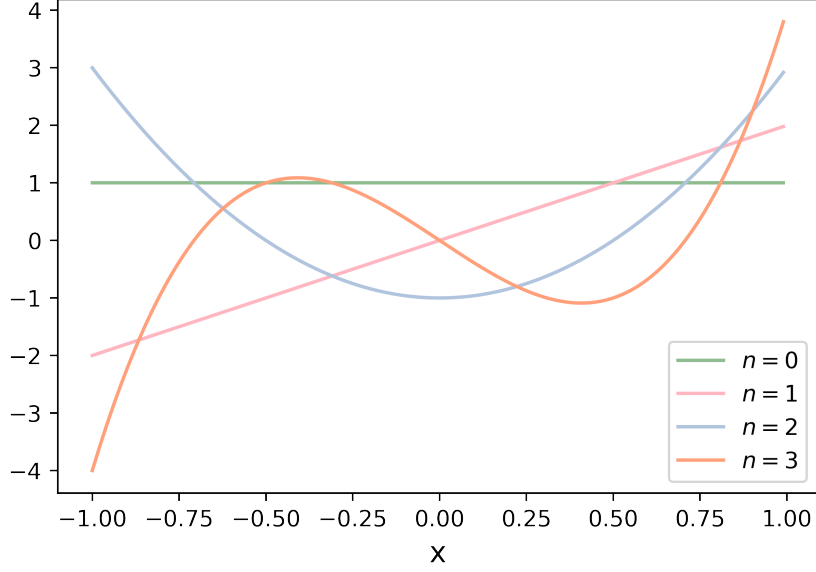


Figure 4.1: The Chebyshev polynomials of second kind of degree $n = 0, 1, 2, 3, 4$.

and $\omega_k = -2x + 2$. We note that the parameters do not depend on the sites of the chain. Thus, they define a homogenous model. It turns out that these parameters are exactly those of the so-called XX model with an external magnetic field $B_n = -2$ [13].

The value of the magnetic field we recover, $B_n = -2$, is a particular value for the XX model. Indeed, it can be shown that when $|B_n| \geq 2$, the ground state is a state where all the spins are aligned. When $|B_n| < 2$, the ground state is in a combination of up and down spins. This abrupt change in the nature of the ground state indicates a quantum phase transition at $B_n = \pm 2$ [35]. We wish to study the XX model with no magnetic field. To achieve this, we add a constant term to the magnetic field term in the Hamiltonian (3.11), $-B_n \rightarrow -B_n - 2$. The Hamiltonian is now given by

$$\hat{H} = - \sum_{n=0}^{N-2} c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n. \quad (4.5)$$

This change only shifts the eigenvalues ω_k that are now given by $\omega_k = -2x$.

Let us now consider the recurrence relation for the eigenfunctions (3.17) for $n = N-1$. Since $J_{N-1} = 0$, we have

$$\omega_k \phi_{N-1,k} = J_{N-2} \phi_{N-2,k}, \quad (4.6)$$

or equivalently, using the mapping to the polynomials (3.70) and the definition of the Chebyshev polynomials (4.1),

$$\begin{aligned} -2x U_{N-1}(x) &= -U_{N-2}(x) \\ \iff 2 \cos \theta \sin((N-1)\theta) &= \sin((N-2)\theta). \end{aligned} \quad (4.7)$$

This relation is satisfied when

$$\theta = \theta_k = \frac{\pi(k+1)}{N+1}, \quad k = 0, \dots, N-1. \quad (4.8)$$

In the following, we write $x_k = \cos \theta_k$. The coefficient w_k is determined such that the orthonormality relation for the eigenfunctions (3.16) is satisfied. Written in terms of the polynomials, the relation is

$$\delta_{kp} = \sum_{n=0}^{N-1} \sqrt{w_k w_p} U_n(x_k) U_n(x_p). \quad (4.9)$$

As the Chebyshev polynomials are defined in terms of sines (4.1), it is possible to evaluate this sum. We find that the relation (4.9) is satisfied if

$$w_k = \frac{2}{N+1} \sin^2(\theta_k). \quad (4.10)$$

The eigenfunctions and the eigenvalues are thus given by

$$\begin{aligned} \phi_{n,k} &= \sqrt{\frac{2}{N+1}} \sin\left(\frac{\pi(k+1)(n+1)}{N+1}\right), \\ \omega_k &= -2 \cos\left(\frac{\pi(k+1)}{N+1}\right). \end{aligned} \quad (4.11)$$

To construct the ground state of the system, we fill the vacuum state with fermions that have negative energies. As we see in Figure 4.2, the energy ω_k is negative in the interval $[0, (N-1)/2]$. If N is even, the ground state is simple and is a state with $f = N/2$ fermions. The energy level of the state is

$$E_0 = \sum_{k=0}^{f-1} \omega_k = 1 - \csc\left(\frac{\pi}{2(N+1)}\right). \quad (4.12)$$

If N is odd, there is one fermion with zero energy as $\omega_{(N-1)/2} = 0$. Therefore, the ground state has a multiplicity of two and is either a state with $f = \lfloor N/2 \rfloor + 1$ or $f = \lfloor N/2 \rfloor$ fermions.¹ The energy is

$$E_0 = \sum_{k=0}^{f-1} \omega_k = 1 - \cot\left(\frac{\pi}{2(N+1)}\right). \quad (4.13)$$

We introduce the filling μ of the state as the ratio between the number of fermions f in the state and the length of the chain N . Therefore, we have

$$\mu = \begin{cases} \frac{1}{2}, & \text{for } N \text{ even,} \\ \frac{N \pm 1}{2N}, & \text{for } N \text{ odd.} \end{cases} \quad (4.14)$$

For both parities of N , the filling tends to $1/2$ as $N \rightarrow \infty$. For that reason, we say that the state is half-filled.

Moreover, from their expression (4.11), we see that the eigenfunctions are symmetric under the exchange of n and k : $\phi_{n,k} = \phi_{k,n}$. In the following, we refer to such

¹Here, $\lfloor \cdot \rfloor$ denotes the floor function.

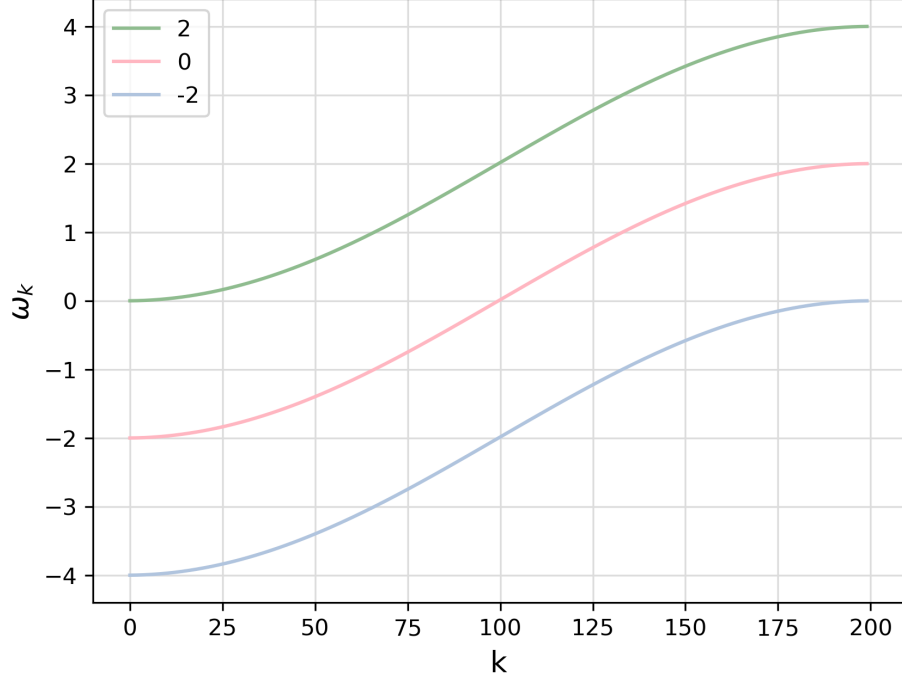


Figure 4.2: The energy ω_k (4.11) as a function of k for different values of the magnetic field for $N = 200$. The case studied here is the no magnetic field case (pink line). The blue and green lines are the energies for the critical value of the magnetic field $B_n = \pm 2$. In these cases, the single particle energy is either always positive or always negative.

a property as a self-duality property. We deduce from the recurrence relation (4.2), with the shifted magnetic field, that the eigenfunctions also satisfy

$$-2\omega_n\phi_{n,k} = -\phi_{n,k+1} - \phi_{n,k-1}, \quad (4.15)$$

and we identify from (3.69),

$$\lambda_n = 2\omega_n = -2\cos\theta_n, \quad \bar{J}_0 = \dots = \bar{J}_{N-2} = -1, \quad \bar{B}_0 = \dots = \bar{B}_{N-1} = 0. \quad (4.16)$$

4.3 Entanglement entropy

In this section, we first study the entanglement of the ground state of the XX model with the entanglement entropy. This topic has been widely studied over the last decades, and many results are already known [9, 13, 21, 36]. We compare those results with our numerical ones in the case of a finite and an infinite system. We then expand the discussion to the first excited state.

4.3.1 Finite system

Using (4.11) in (3.34), we find that the reduced correlation matrix for the XX model is

$$C_{mn} = \left(\frac{2}{N+1}\right) \sum_{k=0}^{f-1} \sin\left(\frac{\pi(k+1)(n+1)}{N+1}\right) \sin\left(\frac{\pi(k+1)(m+1)}{N+1}\right), \quad (4.17)$$

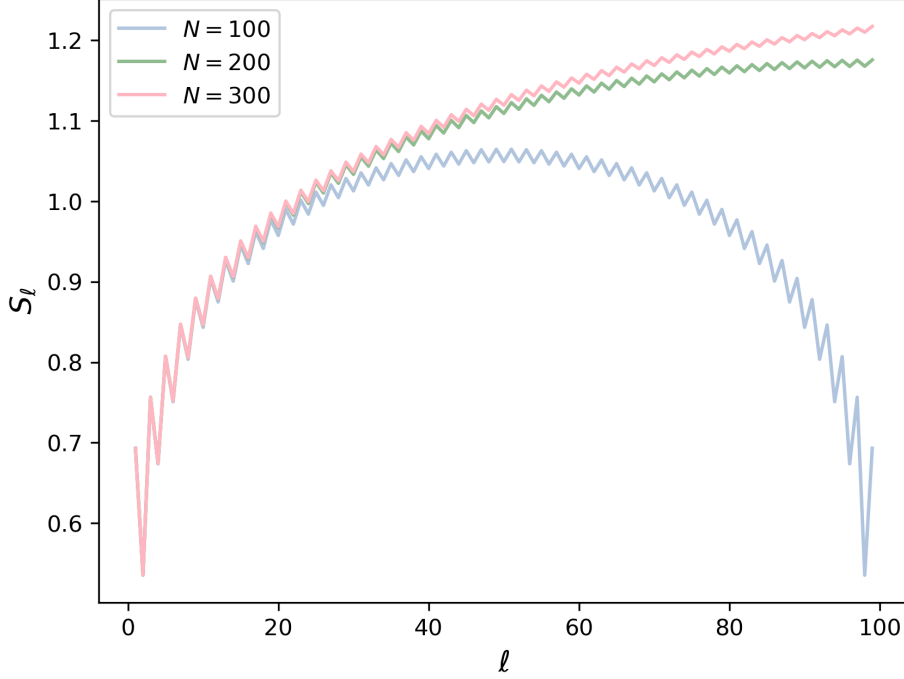


Figure 4.3: The entanglement entropy as a function of the length ℓ of the subsystem for different values of N .

for $m, n = 0, \dots, \ell - 1$. Moreover, we find the commuting matrix T using (3.86), (4.11) and (4.16),

$$\begin{cases} t_n = 2(\cos \theta_n + \cos \theta_{n+1} - \cos \theta_{\ell-1} - \cos \theta_\ell) \\ d_n = -4 \cos \theta_n (\cos \theta_{f-1} + \cos \theta_f) \end{cases} \quad (4.18)$$

Numerical simulations allow us to study the entanglement entropy of the XX model. To compute the entropy, we only need to find the eigenvalues of the correlation matrix and then use the formula (3.47). We use two methods to compute the eigenvalues numerically. The first one is directly from the correlation matrix (4.17). The second one is computing first the eigenvectors of the commuting matrix (4.18) and then acting with them on the correlation matrix to find the eigenvalues. Both methods give the same results, as expected. The time needed for the numerical simulations is similar in both cases. It is thus not clear whether the commuting matrix method has any advantages numerically. Note that the systems we considered here only go up to $N = 300$ and $\ell = 100$. The advantages of the commuting matrix might appear when considering much larger systems. For instance, it could speed up the numerical simulations since the diagonalisation of the commuting matrix is easier than the one for the correlation matrix.

The Figure 4.3 shows the entanglement entropy for different values of N . We see that the entropy is symmetric with respect to the $\ell = N/2$ axis. Thus, the entropy is maximal when the subsystem is half the size of the system. We also notice oscillations due to the parity of the length of the subsystem. We discuss this feature in more detail in Section 4.3.2.

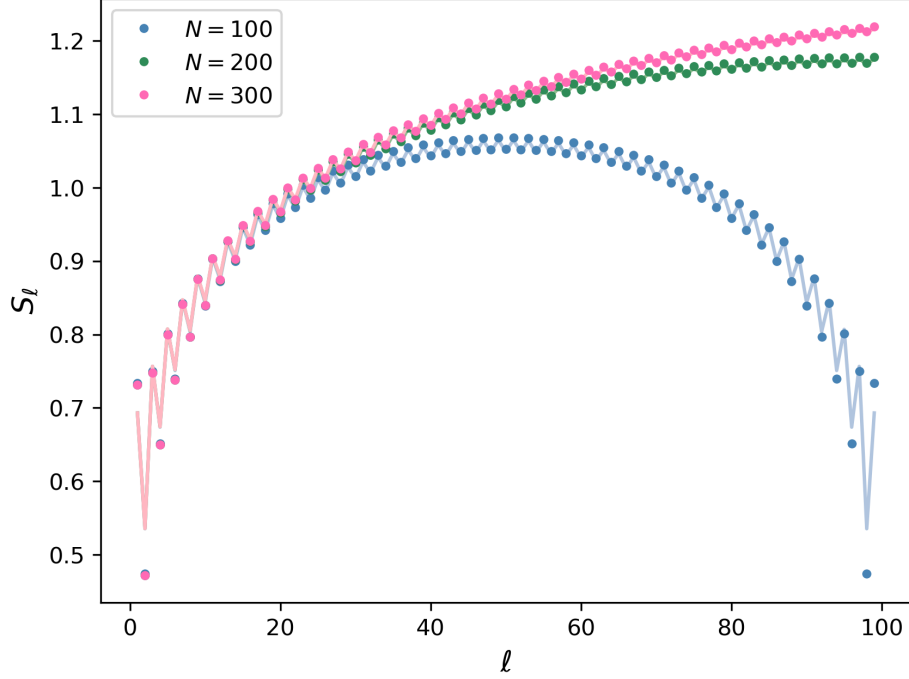


Figure 4.4: This figure shows the entanglement entropy for the XX chain for different values of N . The lighter and continuous lines are the numerical results. The darker and dotted lines are the prediction (4.20). The additive constant is computed from a fit and is $a = 0.4793 \pm 10^{-3}$.

It is also possible to study the entanglement entropy using CFT. Calabrese and Cardy found a prediction for the leading term of the entropy for a block of length ℓ in a chain of finite length N [21]

$$S_\ell = \frac{1}{6} \log \left(\frac{N}{\pi} \sin \left(\frac{\pi \ell}{N} \right) \right) + a + o(1), \quad (4.19)$$

where a is a non-universal constant that we determine using a fit. Its value is given in Figure 4.4.² The oscillating behaviour is described by the subleading terms of the entropy. We recover their expression from [36] and write the entropy as

$$S_\ell = \frac{1}{6} \log \left(\frac{N}{\pi} \sin \left(\frac{\pi \ell}{N} \right) \right) + a - \frac{1}{4} \sin \left(\frac{\pi}{2} (2\ell + 1) \right) \left(\frac{N}{\pi} \sin \left(\frac{\pi \ell}{N} \right) \right)^{-1} + o(N^{-1}). \quad (4.20)$$

In Figure 4.4, we compare our numerical results with the expression (4.20) and see that they coincide.

²We recall that the numerical results are written as stated in the introduction: $a \pm \sigma$ where a is the coefficient computed from the fit and σ is the order of the standard deviation for a . We round up a after the order of the standard deviation. If the order is larger than 10^{-4} , we round up after four decimal places.

4.3.2 Infinite system

We now study the case of a chain of infinite length, $N \rightarrow \infty$. In this limit, the reduced correlation matrix (4.17) becomes

$$C_{mn} = \begin{cases} \frac{\sin\left(\frac{\pi}{2}(m-n)\right)}{\pi(m-n)} - \frac{\sin\left(\frac{\pi}{2}(m+n+2)\right)}{\pi(m+n+2)}, & \text{when } m \neq n, \\ \frac{1}{2} - \frac{\sin(\pi(n+1))}{2\pi(n+1)}, & \text{when } m = n. \end{cases} \quad (4.21)$$

On the one hand, we notice that the first terms of (4.21) define a Toeplitz matrix, *i.e.*, the descending diagonals are constant. On the other hand, we see that the second terms define a Hankel matrix, *i.e.*, the ascending diagonals are constant. The Hankel part of the matrix is a consequence of the open boundary conditions [36]. For periodic boundary conditions, the correlation matrix is defined only by the Toeplitz part [13]. This form of the matrix is convenient as it allows one to determine the asymptotic behaviour of the entropy using methods based on the Fisher-Hartwig conjecture [36]. As in the finite chain case, it is also possible to study the entropy for the infinite chain using CFT [21]. The entropy for a subsystem of length ℓ is, taking into account the oscillating term,

$$S_\ell = \frac{1}{6} \log \ell + a - \frac{1}{4} \sin\left(\frac{\pi}{2}(2\ell+1)\right) \frac{1}{\ell} + o(\ell^{-1}), \quad (4.22)$$

where a is a constant. The entropy thus diverges as the logarithm of the subsystem's size. The parity oscillations are still present. The comparison of our numerical results and (4.22) is shown in Figure 4.5a. In Figure 4.5b, we compare our results and a logarithmic fit, $S_{\text{fit}} = b \log \ell + a$, for subsystems up to $\ell = 300$. We find that the coefficients are given by

$$b = 0.1661 \pm 10^{-4}, \quad a = 0.4793 \pm 10^{-3} \quad (4.23)$$

The multiplicative factor is indeed $1/6$, as predicted in (4.22), up to a relative error of the order of 10^{-3} .

Subleading terms

In both the finite and infinite cases, we see parity oscillations in the behaviour of the entropy. This particular feature is a consequence of the boundary conditions and appears in the subleading terms of the asymptotic expansion [36]. For periodic boundary conditions, the entropy does not exhibit parity oscillations [13]. The entropy for both parities in the infinite case is represented in Figure 4.6. We find numerically that both cases follow the leading term of (4.22) with a relative error for the multiplicative factor of the order of 10^{-3} for the even case and of the order of 10^{-2} for the odd case.

To further analyse the subleading contributions, we compute the difference between our numerical results for the entropy and (4.22) for even and odd lengths. For both cases, we see in Figure 4.7 that the difference tends to zero as ℓ increases. Keeping that observation in mind, we use the function $f(\ell) = b\ell^{-c}$ to fit both cases. The coefficients are given by

- Even case: $b = -0.1596 \pm 10^{-4}$, $c = 0.992 \pm 10^{-4}$,
- Odd case: $b = 0.3243 \pm 10^{-4}$, $c = 0.9952 \pm 10^{-4}$.

Therefore, this result indicates that the parity oscillations attenuate as the subsystem size increases. This conclusion is in agreement with the known expression for the oscillations (4.22).

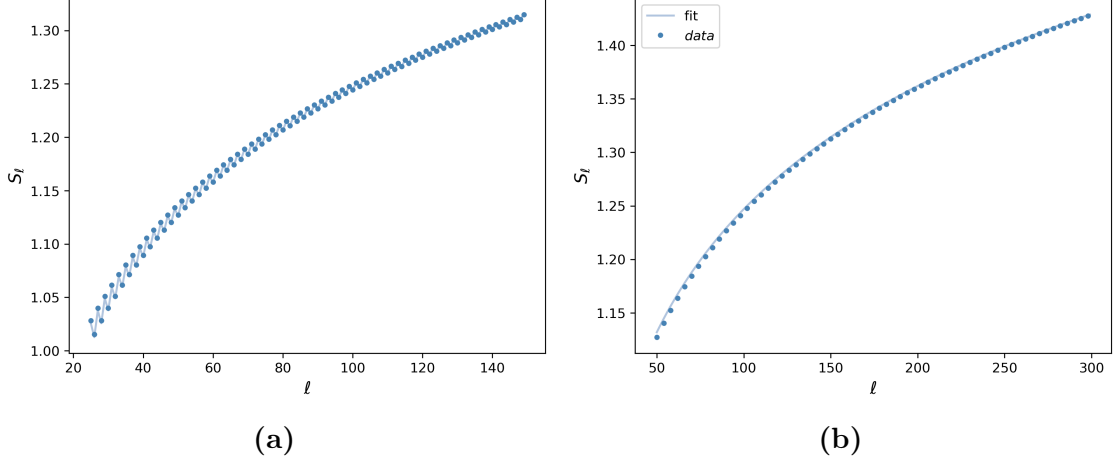


Figure 4.5: (a) The dotted and darker lines are our numerical results for the entropy of the XX model. The continuous and darker lines are the CFT prediction (4.22). (b) The dotted and darker lines are our numerical results for the entanglement entropy of the XX model. The continuous and lighter lines are a logarithmic fit with coefficients (4.23).

4.3.3 Entropy in the first excited state

Up to now, we have only studied entanglement in the ground state of the model. A natural extension to the discussion is to consider the first excited state. It is the eigenstate of the Hamiltonian with eigenvalue E_1 such that $E_0 < E_1 < E_2 < \dots$. We denote by $\tilde{f}$ the number of fermions in this state.

Recall that the single particle energy ω_k (4.11) is symmetric with respect to the $(N-1)/2$ axis. If N is even, the first excited is achieved by filling the vacuum with either $N/2 - 1$ or $N/2 + 1$ fermions and thus has a multiplicity of two. The energy of the state is given by

$$E_1 = \sum_{k=0}^{\tilde{f}-1} \omega_k = 1 - \csc\left(\frac{\pi}{2(N+1)}\right) \cos\left(\frac{\pi}{N+1}\right). \quad (4.24)$$

If N is odd, we have a zero-energy fermion as $\omega_{(N-1)/2} = 0$. Thus, the first excited state is the state filled with either $\lfloor N/2 \rfloor - 1$ or $\lfloor N/2 \rfloor + 2$ fermions. Another possibility is to fill the vacuum with fermions from $k = 0$ to $k = \lfloor N/2 \rfloor + 1$ without taking into account the zero-energy fermion at $k = \lfloor N/2 \rfloor$. We refer to the latter case as a non-compact filling of fermions. Conversely, we refer to the other cases as

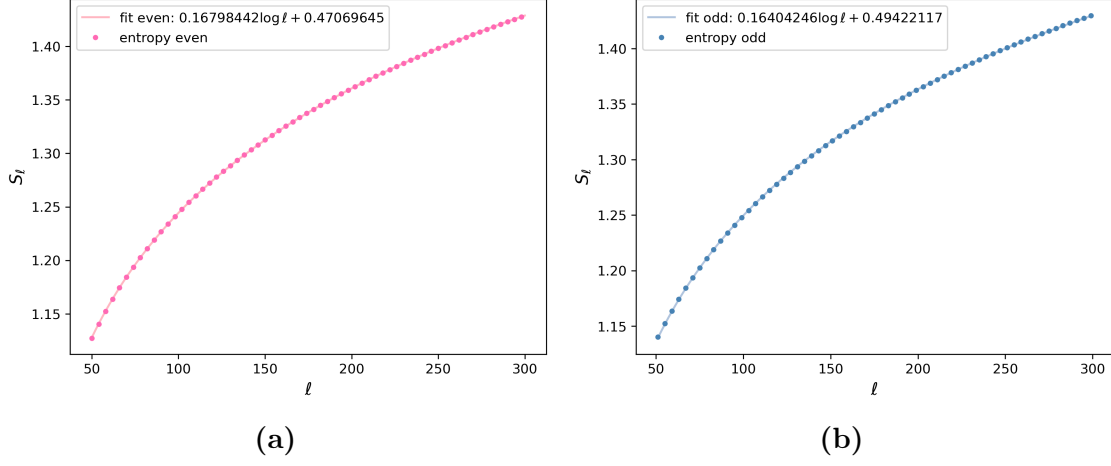


Figure 4.6: This figure shows the entanglement entropy and a fitting curve for (a) even lengths and (b) odd lengths.

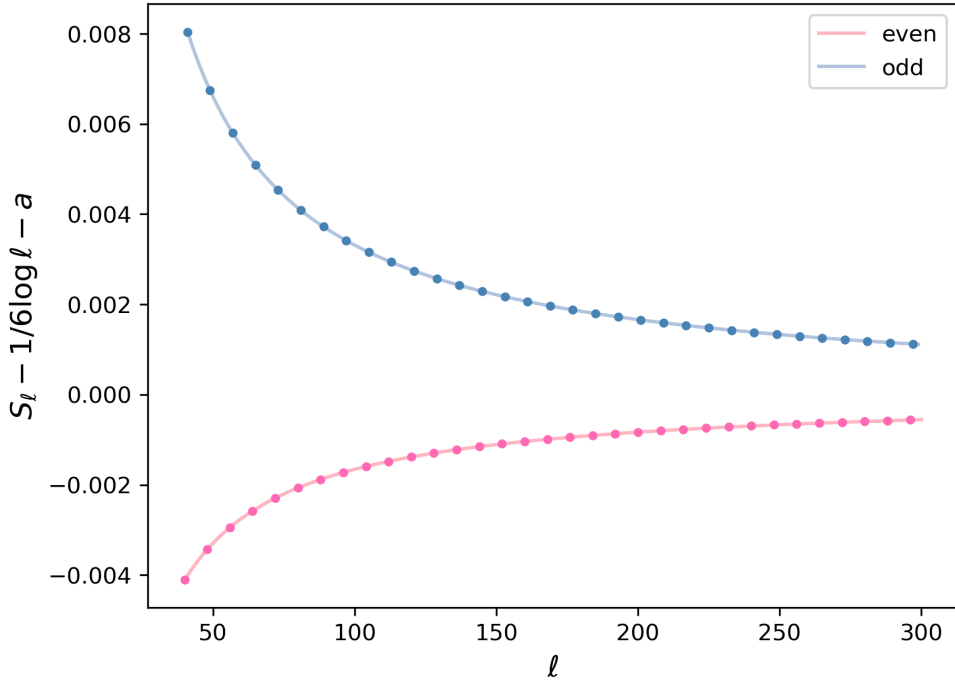


Figure 4.7: This figure shows the difference between the entanglement entropy for the odd and even lengths and the leading term of the entropy (4.22). The continuous and lighter lines are the fits. The dotted and darker lines are the numerical results. The additive constant is found using a fit and is given by $a = 0.4793 \pm 10^{-3}$.

states with a compact filling. The energy is

$$E_1 = \sum_{k=0}^{\tilde{f}-1} \omega_k = 1 - \csc \left(\frac{\pi}{2(N+1)} \right) \cos \left(\frac{3\pi}{N+1} \right). \quad (4.25)$$

For simplicity, we choose to only consider the states with a compact filling. The first

excited state is defined as

$$|\psi_1\rangle = \prod_{k=0}^{\tilde{f}-1} d_k^\dagger |0\rangle. \quad (4.26)$$

The procedure to find the entropy is similar to the ground state case with $\tilde{f}$ instead of f . The other variables, N and ℓ , are the same. Thus, the only changes appear in the correlation matrix where we sum over the occupied fermions. We choose $\tilde{f} = \lfloor N/2 \rfloor - 1 = f - 1$ to illustrate the discussion. The arguments are similar for other choices of $\tilde{f}$ as they can all be written in terms of f . The reduced correlation matrix in the first excited $\tilde{C}$ is related to the one in the ground state C as

$$\begin{aligned} \tilde{C}_{mn} &= \frac{2}{N+1} \sum_{k=0}^{\tilde{f}-1} \sin\left(\frac{\pi(n+1)(k+1)}{N+1}\right) \sin\left(\frac{\pi(m+1)(k+1)}{N+1}\right) \\ &= C_{mn} - \frac{2}{N+1} \sin\left(\frac{\pi(n+1)f}{N+1}\right) \sin\left(\frac{\pi(m+1)f}{N+1}\right), \end{aligned} \quad (4.27)$$

with $m, n = 0, \dots, \ell$. For finite N , the entropy is represented in Figure 4.8. The leading behaviour of the entropy is the same as in the ground state (4.19) with the same additive constant. The only difference is the behaviour of the oscillations. The excited particle contributes to a term in $1/N$ in the correlation matrix. Therefore, in the limit of a large system, the second term of (4.27) vanishes, and we have

$$\lim_{N \rightarrow \infty} \tilde{C}_{mn} = C_{mn}. \quad (4.28)$$

In this limit, the entropy in the first excited state is equal to the entropy in the ground state. As the only change is the number of fermions, one may also see the first excited state as the ground state of an XX model with an appropriate magnetic field [37]. It is thus not a surprise that the entropy exhibits the same logarithmic behaviour in the limit of a large system. Some changes appear if we consider higher excited states. The entropy for those states still follows the same logarithmic behaviour but the additive constant changes [37].

4.3.4 Conclusion

The XX model is one of the easiest models of quantum magnetism. Therefore, it is the perfect starting point for our investigations. Here, we have constructed the model from the Chebyshev polynomials of the second kind, using the formalism introduced in the previous chapter. We recovered exactly all of the already-known quantities for the XX model. This method eases the calculations as, for instance, one does not have to diagonalise the matrix H by hand but can recover the results directly from the polynomial theory of Chapter 2.

In this section, we have studied the entanglement entropy for the model with open boundary conditions. This quantity has been widely studied over the years, and many results are known and celebrated, especially from CFT. We found out that our numerical simulations were in excellent agreement with these results in both the finite and infinite system's size cases.

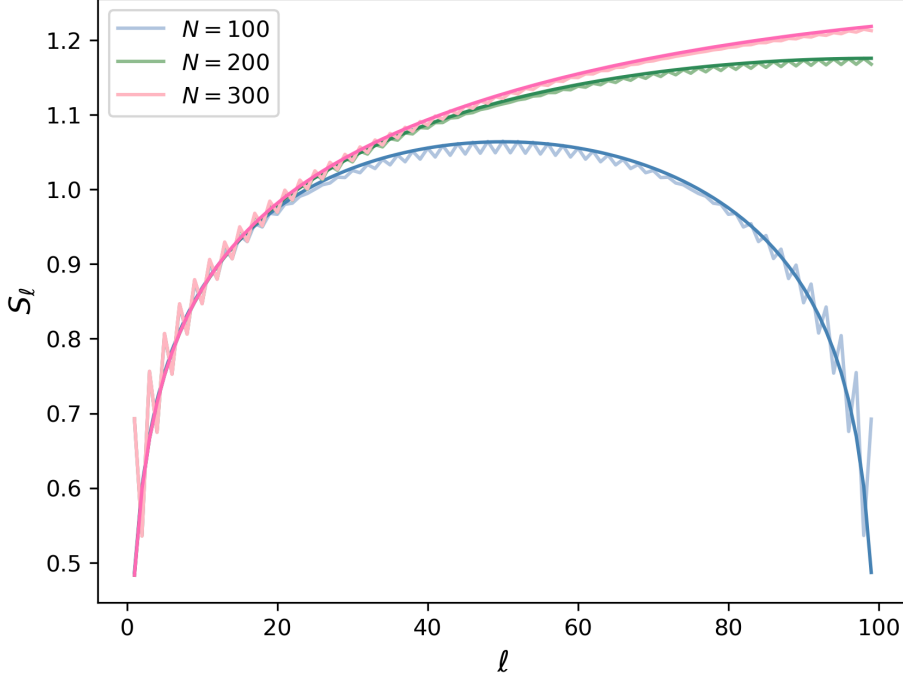


Figure 4.8: The entropy in the first excited state for $N = 100, 200, 300$. The lighter lines are the numerical results. The darker lines are the CFT prediction (4.19).

We then expanded the discussion to consider the first excited state of the system. We have only considered states with compact fillings of fermions. It is worth studying states with non-compact fillings. Numerical simulations showed that, for finite N , the entropy for that case does not follow (4.19) and a correction to this prediction is needed. However, in the limit $N \rightarrow \infty$, the correction vanishes, and we once again recover the reduced correlation matrix of the ground state and, thus, the same entropy. It would be interesting to characterise this change. This has been done for periodic boundary conditions using CFT in [38]. In the limit $N \rightarrow \infty$, higher excited states follow the logarithmic behaviour of the ground state up to an additive constant, regardless of the compactness of the filling [37].

4.4 Bipartite fidelity

We now move on to the study the bipartite fidelity of the XX model. This section is based on Stéphan's Ph.D. thesis [15] and Parez's master's thesis [39]. Recall that for the bipartite fidelity, one has to study first the whole system and then the system divided into two independent subsystems A and B . Note that this bipartition is different from the one we made in the study of the entropy, as the two subsystems were not independent in that case.

Most of the work for the whole system has already been done in previous sections. We recall some results that will be useful, now using the usual notations for the bipartite fidelity introduced in Section 2.2. The Hamiltonian for the whole

system $A \cup B$ is

$$\hat{H} = \sum_{k=0}^{N-1} \omega_k d_k^\dagger d_k, \quad \omega_k = -2 \cos \left(\frac{\pi(k+1)}{N+1} \right), \quad (4.29)$$

and the fermionic operators

$$\begin{aligned} d_k &= \left(\frac{2}{N+1} \right)^{1/2} \sum_{j=0}^{N-1} \sin \left(\frac{\pi(k+1)(j+1)}{N+1} \right) c_j, \\ d_k^\dagger &= \left(\frac{2}{N+1} \right)^{1/2} \sum_{j=0}^{N-1} \sin \left(\frac{\pi(k+1)(j+1)}{N+1} \right) c_j^\dagger. \end{aligned} \quad (4.30)$$

The ground state is filled with f fermions and it is defined as

$$|A \cup B\rangle = \prod_{k=0}^{f-1} d_k^\dagger |0\rangle. \quad (4.31)$$

4.4.1 Two subsystems

To compute the bipartite fidelity, we have to construct the ground state of the system when it is composed of two independent subsystems A and B . We consider N_A (resp. N_B) spins in the subsystem A (resp. B) such that $N = N_A + N_B$. The Hamiltonian is given by

$$\hat{H}_{A \otimes B} = \underbrace{-\frac{1}{2} \sum_{j=0}^{N_A-2} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y)}_{\hat{H}_A} - \underbrace{\frac{1}{2} \sum_{j=N_A}^{N-2} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y)}_{\hat{H}_B}. \quad (4.32)$$

To construct this Hamiltonian, we have only switched off the interaction between A and B in the whole system. After the Jordan-Wigner transformation, we have

$$\hat{H}_{A \otimes B} = \sum_{i,j=0}^{N-1} H_{ij}^{A \otimes B} c_i^\dagger c_j, \quad (4.33)$$

with the matrix $H^{A \otimes B}$ is a $N \times N$ matrix defined as

$$H^{A \otimes B} = \begin{pmatrix} H^A & 0 \\ 0 & H^B \end{pmatrix}. \quad (4.34)$$

Here, H^A (resp. H^B) is the $N_A \times N_A$ matrix (resp. $N_B \times N_B$) associated with the Hamiltonian $\hat{H}_A$ (resp. $\hat{H}_B$). The diagonalisation yields

$$\hat{H}_{A \otimes B} = \sum_{j=0}^{N-1} \gamma_j s_j^\dagger s_j, \quad (4.35)$$

with

$$s_j = \begin{cases} \left(\frac{2}{N_A + 1} \right)^{1/2} \sum_{k=0}^{N_A-1} \sin \left(\frac{\pi(k+1)(j+1)}{N_A + 1} \right) c_k, & 0 \leq j \leq N_A - 1, \\ \left(\frac{2}{N_B + 1} \right)^{1/2} \sum_{k=0}^{N_B-1} \sin \left(\frac{\pi(k+1)(j+1-N_A)}{N_B + 1} \right) c_{k+N_A}, & N_A \leq j \leq N - 1, \end{cases} \quad (4.36)$$

and

$$\gamma_j = \begin{cases} -2 \cos \left(\frac{\pi(j+1)}{N_A + 1} \right), & 0 \leq j \leq N_A - 1, \\ -2 \cos \left(\frac{\pi(j+1-N_A)}{N_B + 1} \right), & N_A \leq j \leq N - 1. \end{cases} \quad (4.37)$$

The operators s_j are fermionic operators acting either in subsystem A or B .

Let us now define the ground state $|A \otimes B\rangle$. The number of fermions in the ground state of $A \otimes B$ must be equal to the number of fermions in $A \cup B$. Indeed, if the states have different numbers of fermions, they correspond to eigenvectors of the number operator with different eigenvalues. They are thus orthogonal, and the bipartite fidelity vanishes. We consider f_A and f_B fermions in subsystems A and B , respectively, such that $f = f_A + f_B$. The ground state is then

$$|A \otimes B\rangle = \prod_{i=0}^{f_A-1} s_i^\dagger \prod_{j=N_A}^{N_A+f_B-1} s_j^\dagger |0\rangle = \prod_{i=0}^{f-1} \tilde{s}_i^\dagger |0\rangle, \quad (4.38)$$

with

$$\tilde{s}_j = \begin{cases} s_j, & 0 \leq j \leq f_A - 1 \\ s_{N_A+j-f_A}, & f_A \leq j \leq f - 1. \end{cases} \quad (4.39)$$

The parity of the lengths of the subsystems influences the parity of the system's length. At half-filling, we consider three configurations for the lengths of the subsystems:

- Even-even: $N = 2f$, $N_{A,B} = 2f_{A,B}$,
- Odd-odd: $N = 2f$, $N_A = 2f_A + 1$, $N_B = 2f_B - 1$,
- Odd-even: $N = 2f - 1$, $N_A = 2f_A - 1$, $N_B = 2f_B$.

The multiplicity of the ground state depends on the parity of the length of the subsystems. If N_A and N_B are both even, the ground state is simple. If N_A and N_B are odd, the ground state has a multiplicity of four. If N_A and N_B have different parities, the ground state has a multiplicity of two.

4.4.2 Bipartite fidelity

Using (2.16), (4.31) and (4.38), we write the bipartite fidelity for the XX model as

$$\mathcal{B} = \left| \langle 0 | \prod_{j=0}^{f-1} \tilde{s}_{f-1-j} \prod_{k=0}^{f-1} d_k^\dagger | 0 \rangle \right|^2. \quad (4.40)$$

By means of Wick's theorem [28], it is possible to write this product as a determinant of two-point functions. The bipartite fidelity is then given by

$$\mathcal{B} = \left| \det_{0 \leq i, j \leq f-1} \langle 0 | \tilde{s}_i d_j^\dagger | 0 \rangle \right|^2 = |\det \mathcal{M}|^2. \quad (4.41)$$

Using the definition of the $d_j^\dagger$ (4.30) and the $\tilde{s}_i$ (4.36) operators, it is possible to write the matrix elements as a sum and to calculate it exactly. Therefore, we find that $\mathcal{M}$ is a $f \times f$ matrix defined by

$$\mathcal{M}_{ij} = \begin{cases} \frac{(-1)^{i+1}}{\sqrt{(N_A+1)(N+1)}} \frac{\sin\left(\frac{(i+1)\pi}{N_A+1}\right) \sin\left(\frac{\pi(j+1)(N_A+1)}{N+1}\right)}{\cos\left(\frac{(i+1)\pi}{N_A+1}\right) - \cos\left(\frac{(j+1)\pi}{N+1}\right)}, & 0 \leq i \leq f_A - 1, \\ \frac{-1}{\sqrt{(N_B+1)(N+1)}} \frac{\sin\left(\frac{(i+1-f_A)\pi}{N_B+1}\right) \sin\left(\frac{\pi(j+1)N_A}{N+1}\right)}{\cos\left(\frac{(i+1-f_A)\pi}{N_B+1}\right) - \cos\left(\frac{(j+1)\pi}{N+1}\right)}, & f_A \leq i \leq f - 1. \end{cases} \quad (4.42)$$

This expression holds for all N_A, N_B unless

$$\frac{i+1}{N_A+1} = \frac{j+1}{N+1} \quad \text{or} \quad \frac{i+1-f_A}{N_B+1} = \frac{j+1}{N+1}. \quad (4.43)$$

In that case, the matrix elements are

$$\mathcal{M}_{ij} = \begin{cases} \left(\frac{N_A+1}{N+1}\right)^{1/2}, & 0 \leq i \leq f_A - 1 \quad \text{and} \quad \frac{i+1}{N_A+1} = \frac{j+1}{N+1}, \\ (-1)^{j-i+f_A} \left(\frac{N_B+1}{N+1}\right)^{1/2}, & f_A \leq i \leq f - 1 \quad \text{and} \quad \frac{i+1-f_A}{N_B+1} = \frac{j+1}{N+1}. \end{cases} \quad (4.44)$$

Closed form of the bipartite fidelity

For the specific choice of parameters $N = 2N_{A,B}$ and $f = 2f_{A,B}$ with f even, it is possible to find a closed form of the bipartite fidelity. Note that with that choice, the cases (4.43) are never satisfied. The matrix elements of $\mathcal{M}$ are then given by

$$\mathcal{M}_{ij} = \begin{cases} (-1)^{i+1} \frac{a_i b_j}{x_i + y_j}, & 0 \leq i \leq f/2 - 1, \\ (-1)^{j+1} \frac{a_{i-f/2} b_j}{x_{i-f/2} + y_j}, & f/2 \leq i \leq f - 1, \end{cases} \quad (4.45)$$

with

$$\begin{aligned} a_i &= \frac{1}{\sqrt{N/2+1}} \sin \theta_i, & b_j &= \frac{1}{\sqrt{N+1}} \sin \left(\frac{j+1}{2} + \frac{\phi_j}{2} \right), \\ x_i &= \cos \theta_i, & y_j &= -\cos \phi_j, \end{aligned} \quad (4.46)$$

and

$$\theta_i = \frac{(i+1)\pi}{N/2+1}, \quad \phi_j = \frac{(j+1)\pi}{N+1}. \quad (4.47)$$

This matrix has similarities with the so-called Cauchy matrices, for which a closed form of the determinant is known [40]. In our case, it is possible to use similar techniques and to also find a closed form for the determinant [15]. A detailed derivation is presented in the appendix of Parež's master thesis [39]. We obtain

$$\det \mathcal{M} = \prod_{i=0}^{f/2-1} \left[\sin^2 \theta_i \prod_{j=i+1}^{f/2-1} (\cos \theta_i - \cos \theta_j)^2 \right] \prod_{j=0}^{f-1} \sin \left(\frac{(j+1)\pi}{2} + \frac{\phi_j}{2} \right) \times \frac{\prod_{\substack{(i-j)\text{even} \\ 0 \leq i, j \leq f-1}} (\cos \phi_i - \cos \phi_j)}{2^{-f/2} [(N+1)(N/2+1)]^{f/2} \prod_{i=0}^{f/2-1} \prod_{j=0}^{f-1} (\cos \theta_i - \cos \phi_j)}. \quad (4.48)$$

We now write the logarithmic bipartite fidelity using its definition (2.17). It is interesting to study the behaviour of the LBF in the limit of a large system, as done in the appendix of Stéphan's thesis [15]. At half-filling, he finds that the leading term of the asymptotic expansion is given by

$$\mathcal{F} = \frac{1}{8} \log N + a + o(1), \quad \text{as } N \rightarrow \infty, \quad (4.49)$$

where a is a constant that we determine numerically in the following section.

4.4.3 Numerical results

In this section, we compare our numerical results for the bipartite fidelity and the asymptotic expansion (4.49). As before, we consider f even. We are interested in the following configurations:

- Even-even: $N = 2f$, $N_A = N_B = f$,
- Odd-odd: $N = 2f$, $N_A = f + 1$, $N_B + 1 = f - 1$,
- Even-odd: $N = 2f - 1$, $N_A = f$, $N_B = f - 1$.

We compute the determinant of the matrix defined by (4.42) and (4.44) and obtain the logarithmic bipartite fidelity for each configuration as shown in Figure 4.9. We see that it has indeed a logarithmic behaviour, as proven analytically by (4.49).

For more precise results, we take into account the subleading terms of the asymptotic expansion [15] and fit our numerical results with

$$\mathcal{F}_{\text{fit}} = a_1 \log N + a_2 + a_3 \frac{\log N}{N} + a_4 \frac{1}{N}. \quad (4.50)$$

For systems up to $N = 600$, we find

- Even-even: $a_1 = 0.1250059 \pm 10^{-7}$, $a_2 = -0.1261103 \pm 10^{-7}$,
 $a_3 = 0.13124 \pm 10^{-5}$, $a_4 = 0.0213 \pm 10^{-4}$,
- Odd-odd: $a_1 = 0.1249850 \pm 10^{-7}$, $a_2 = 0.567219 \pm 10^{-6}$,
 $a_3 = -0.39062 \pm 10^{-5}$, $a_4 = 0.6691 \pm 10^{-4}$,

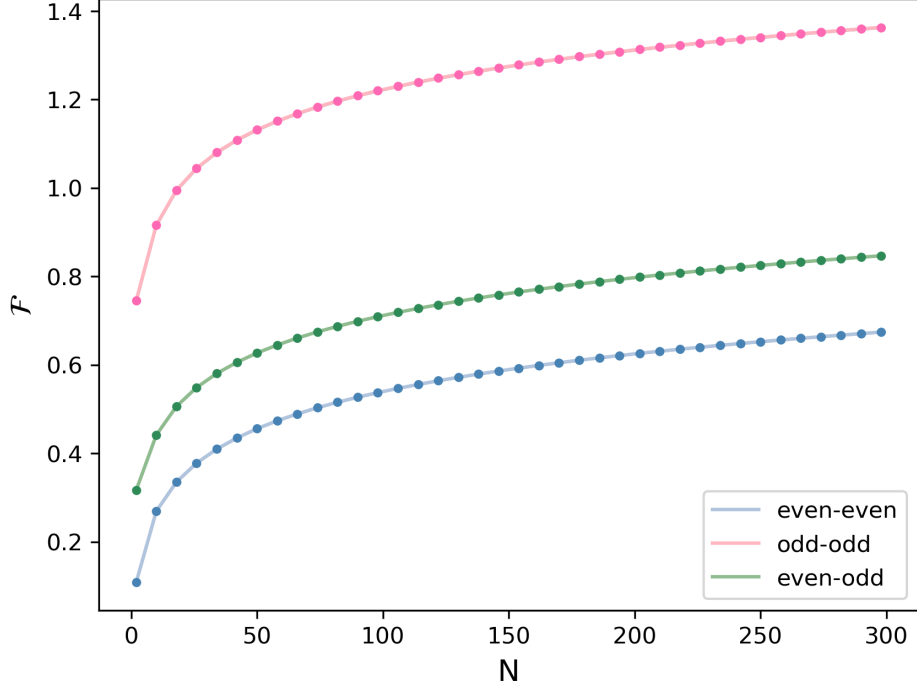


Figure 4.9: This figure shows the LBF as a function of N for each configuration. The dotted and darker lines are the numerical results. The lighter and continuous lines are the numerical fits.

- Even-odd: $a_1 = 0.1250055 \pm 10^{-7}$, $a_2 = 0.047181 \pm 10^{-6}$,
 $a_3 = 0.00503 \pm 10^{-5}$, $a_4 = 0.3829 \pm 10^{-4}$.

The coefficients for the even-even case were computed analytically in [15]. We compare the results we find numerically with them. We get $a_1 = 1/8$ up to a relative error of the order of 10^{-5} . Note that this result is also valid for the other configurations with a relative error of 10^{-5} for the even-odd case and of the order of 10^{-4} for the odd-odd one. The additive constant a_2 is known from Stéphan's asymptotic analysis [15] and is equal to $a_2 = -\log C$ with $C = 1.134348$. Our numerical results give the same result up to a relative error of the order of 10^{-4} . We also get $a_3 = 1/8$ up to a relative order of the order of 10^{-2} . Note that we only considered systems up to $N = 600$. In his thesis [15], Stéphan considered larger systems for the numerical analysis and was able to match the theoretical results with more accuracy.

Subleading terms

Let us now investigate the subleading terms of the bipartite fidelity as a function of $x = N_A/N$ for fixed N . We compare our numerical results with the CFT prediction (2.18). We first compute the conformal weights h_i , $i = 1, \dots, 4$, that appear in (2.19).

The weights h_i , $i = 1, 3, 4$, are associated with the systems of lengths N_A , N_B and N respectively. To find them, we expand the energy of the ground state for even (4.12) and odd (4.13) lengths for large N . Then we compare the results with the expression of finite-size scaling of the energy (2.20). For the XX model, the central

charge is $c = 1$ [41] and the Fermi velocity is $\nu_F = 2 \sin(\mu\pi)$ where $\mu = f/N$ is the filling fraction [15]. We obtain that the weights are given by

$$h_{\text{even}} = 0, \quad h_{\text{odd}} = 1/8. \quad (4.51)$$

As $c = 1$, the relation $\sum_{i=1}^4 \alpha_i = 0$ holds and allows us to find the coefficients α_i , $i = 1, \dots, 4$ for each configuration

- Even-even: $\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 0$,
- Odd-odd: $\alpha_1 = -\alpha_3 = 1/2, \quad \alpha_2 = \alpha_4 = 0$,
- Even-odd: $\alpha_1 = \alpha_2 = 0, \quad \alpha_3 = -\alpha_4 = 1/2$.

We note that we always have $h_2 = 0$. Hence, we recover the $1/8$ leading coefficient in (2.18). In Figure 4.10, we compare our numerical results with the CFT prediction (2.18). We choose $N = 100$ for the even-even and odd-odd cases and $N = 99$ for the even-odd case. The functions $f(x)$ and $g(x)$ from (2.19) are computed with the coefficients (4.51) and are defined up to an additive and a multiplicative constant, respectively. For the three configurations, we compute them numerically and obtain

- Even-even: $\xi_f = 0.1083 \pm 10^{-4}, \quad \xi_g = 0.6097 \pm 10^{-2}$,
- Odd-odd: $\xi_f = 0.0942 \pm 10^{-4}, \quad \xi_g = 0.18029 \pm 10^{-5}$,
- Even-odd: $\xi_f = 0.1075 \pm 10^{-4}, \quad \xi_g = 0.5733 \pm 10^{-2}$.

As we see in Figure 2.18, the numerical results are in agreement with the theory. These constants could be found more precisely considering larger system sizes. They should also be accessible analytically with asymptotic analysis. This process is, however, quite demanding, and the asymptotic development of the subleading terms of the LBF is highly non-trivial [15].

4.4.4 Bipartite fidelity in the first excited state

In this section, we expand the discussion to include the first excited state of the XX model. Recall that we defined that state in Section 4.3.3. For simplicity, we only consider states with compact fillings of fermions. Let $\tilde{f}$, $\tilde{f}_A$ and $\tilde{f}_B$ be the number of fermions in the states $|A \cup B\rangle$, $|A\rangle$ and $|B\rangle$, respectively, with $\tilde{f} = \tilde{f}_A + \tilde{f}_B$. As the only difference is the number of fermions, the procedure to compute the bipartite fidelity is similar to the ground state one. Hence, the expression of (4.42) still holds, but substituting f , f_A , f_B with $\tilde{f}$, $\tilde{f}_A$, $\tilde{f}_B$.

To investigate the subleading terms, we need to compute the conformal weights associated with the first excited state, h_i^1 , $i = 1, \dots, 4$. In order to find h_i^1 , $i = 1, 3, 4$, we expand the energy for even (4.24) and odd (4.25) lengths for large N . Then we compare it with the finite-size scaling of the energy (2.20), which is also valid for the first excited state [18]. The expansion only depends on the parity of the length of the system considered. We obtain

$$h_{\text{even}}^1 = 1/2, \quad h_{\text{odd}}^1 = 9/8. \quad (4.52)$$

To ensure the same number of fermions in $|A \cup B\rangle$ and $|A \otimes B\rangle$, we consider combinations of first excited states and ground states. In the following, we only investigate two different cases, but many others are possible.

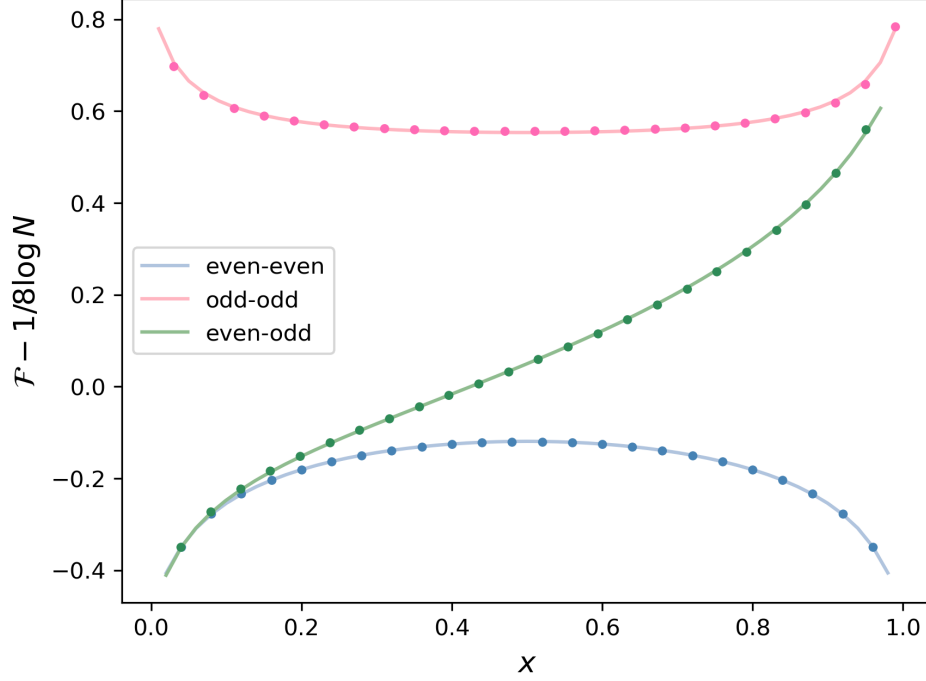


Figure 4.10: This figure shows the difference between the LBF and the leading term of the asymptotic expansion as a function of $x = N_A/N$ for each configuration at half-filling. For the even-even and the odd-odd cases, we consider $N = 100$. For the even-odd case, $N = 99$. The continuous and lighter lines are the CFT predictions. The dotted and darker lines are the numerical results.

Case 1

The first case we consider is the states $|A \cup B\rangle$, $|A\rangle$ in their respective first excited state and $|B\rangle$ in its ground state. As before, we consider $\tilde{f}$ even and $\tilde{f}_A = \tilde{f}_B = \tilde{f}/2$. The different combinations of parities for the lengths are then

- Even-even: $N = 2(\tilde{f} + 1)$, $N_A = \tilde{f} + 2$, $N_B = \tilde{f}$,
- Odd-odd: $N = 2(\tilde{f} + 1)$, $N_A = \tilde{f} + 3$, $N_B = \tilde{f} - 1$,
- Even-odd: $N = 2(\tilde{f} + 1) + 1$, $N_A = \tilde{f} + 2$, $N_B = \tilde{f} + 1$.

We compute numerically the determinant of (4.42) with $\tilde{f}$, $\tilde{f}_A$, $\tilde{f}_B$ and then use the formula (2.17) to compute the LBF. Our results for the LBF as a function of N are shown in Figure 4.11a. We fit our results with

$$\mathcal{F}_{\text{fit}} = a_1 \log N + a_2 + a_3 \frac{\log N}{N} + a_4 \frac{1}{N}. \quad (4.53)$$

We considered systems from $N = 50$ to $N = 600$ in our fits. This is justified as we are studying the asymptotic behaviour of the LBF. The coefficients we obtain are

- Even-even: $a_1 = 0.124737 \pm 10^{-6}$, $a_2 = 0.56934 \pm 10^{-5}$,
 $a_3 = -0.6049 \pm 10^{-3}$, $a_4 = -0.7933 \pm 10^{-3}$,
- Odd-odd: $a_1 = 0.12362 \pm 10^{-5}$, $a_2 = 2.6599 \pm 10^{-4}$,
 $a_3 = -3.0585 \pm 10^{-3}$, $a_4 = -2.8172 \pm 10^{-2}$,

- Even-odd: $a_1 = 0.124897 \pm 10^{-6}$, $a_2 = 0.04811 \pm 10^{-5}$,
 $a_3 = -0.0925 \pm 10^{-4}$, $a_4 = -0.0116 \pm 10^{-3}$.

For each partition, we find that the a_1 term is $1/8$ with a relative error of the order of 10^{-3} for the even-even case, 10^{-2} for the odd-odd case, and 10^{-4} for the even-odd case. We thus recover the same leading behaviour for this configuration as for the ground state (4.49). The other coefficients are, however, different. This indicates some changes in the subleading behaviour.

We now investigate the LBF as a function of $x = N_A/N$ for fixed N . To compare our results with the CFT prediction (2.18), we first determine the coefficients α_i , $i = 1, \dots, 4$. The coefficients $\alpha_{1,4}$ are associated with the first excited states and thus are related to the weights (4.52). As α_3 is associated with a ground state, it is related to the ground state weights (4.51). Moreover, we determine α_2 using the condition $\sum_{i=1}^4 \alpha_i = 0$. For each partition, we have

- Even-even: $\alpha_1 = -\alpha_4 = 1$, $\alpha_2 = \alpha_3 = 0$,
- Odd-odd: $\alpha_1 = -3/2$, $\alpha_2 = 0$, $\alpha_3 = 1/2$, $\alpha_4 = 1$,
- Even-odd: $\alpha_1 = -1$, $\alpha_2 = 0$, $\alpha_3 = -1/2$, $\alpha_4 = 3/2$.

For each case, we have $\alpha_2 = 0$. Hence, we always have $h_2 = 0$ and the leading coefficient of the LBF is $1/8 \log N$ as was the case for the ground state. The multiplicative and additive constants of the functions $f(x)$ and $g(x)$ are computed numerically. We find

- Even-even: $\xi_f = 0.1042 \pm 10^{-3}$, $\xi_g = 0.467 \pm 10^{-2}$,
- Odd-odd: $\xi_f = 0.0504 \pm 10^{-2}$, $\xi_g = 0.2091 \pm 10^{-2}$,
- Even-odd: $\xi_f = 0.1005 \pm 10^{-3}$, $\xi_g = 0.4638 \pm 10^{-2}$.

The comparison of our results and the CFT prediction is shown in Figure 4.12b. We see that the behaviour is completely different from the ground state case. However, our results still follow the CFT prediction (2.18).

Case 2

The second case we consider is the states $|A \cup B\rangle$ in its ground state and $|A\rangle$ and $|B\rangle$ in their respective first excited states. The different combinations are, with $\tilde{f}$ even and $\tilde{f}_A = \tilde{f}_B = \tilde{f}/2$,

- Even-even: $N = 2\tilde{f}$, $N_A = \tilde{f} + 2$, $N_B = \tilde{f} - 2$,
- Odd-odd: $N = 2\tilde{f}$, $N_A = \tilde{f} + 3$, $N_B = \tilde{f} - 3$,
- Even-odd: $N = 2\tilde{f} - 1$, $N_A = \tilde{f} + 2$, $N_B = \tilde{f} - 3$.

The LBF as a function of N is shown in Figure 4.12a and compared to the expression (4.53). We only take into account systems from $N = 100$ to $N = 700$ in the numerical simulations. We find that the coefficients are given by

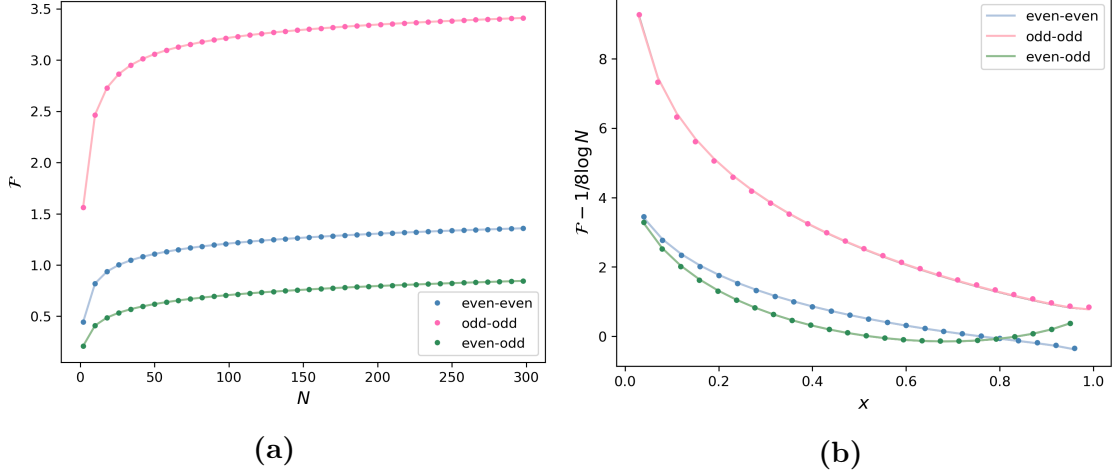


Figure 4.11: These figures show the results for Case 1. **(a)** The LBF as a function of N . The dotted and darker lines are our results and the continuous and lighter lines are the fits. **(b)** The subleading terms are a function of $x = N_A/N$ with $N = 100$ for the even cases and $N = 99$ for the odd one. The dotted and darker lines are our results and the continuous and lighter lines are the CFT predictions.

- Even-even: $a_1 = 0.124802 \pm 10^{-6}$, $a_2 = 2.64829 \pm 10^{-5}$,
 $a_3 = -2.1065 \pm 10^{-3}$, $a_4 = 3.4176 \pm 10^{-3}$,
- Odd-odd: $a_1 = 0.12399 \pm 10^{-5}$, $a_2 = 6.1212 \pm 10^{-4}$,
 $a_3 = -5.5143 \pm 10^{-3}$, $a_4 = 10.8699 \pm 10^{-2}$,
- Even-odd: $a_1 = 0.124571 \pm 10^{-6}$, $a_2 = 4.20989 \pm 10^{-5}$,
 $a_3 = -3.4467 \pm 10^{-3}$, $a_4 = 14.2074 \pm 10^{-2}$.

We see that the leading coefficient a_1 is again $1/8$ up to a relative error of the order of 10^{-3} for each partition. The differences appear in the other coefficients. In particular, we notice that the LBF takes much higher values than in the ground state case. Recalling the interpretation of the (logarithmic) bipartite fidelity, this means that the subsystems in their excited states are less similar to the ground state of the whole system than the subsystems in their ground states are.

We now study the LBF as a function of $x = N_A/N$ for fixed N . The coefficients $\alpha_{1,3}$ are both associated with excited states and thus are related to the weights (4.52). The coefficient α_4 is associated with a ground state and is related to the weights (4.51). Using the relation $\sum_{i=1}^4 \alpha_i = 0$ to determine α_2 , we have for each partition

- Even-even: $\alpha_1 = -\alpha_3 = 1$, $\alpha_2 = \alpha_4 = 0$,
- Odd-odd: $\alpha_1 = -\alpha_3 = 3/2$, $\alpha_2 = \alpha_4 = 0$,
- Even-odd: $\alpha_1 = 1$, $\alpha_2 = 0$, $\alpha_3 = -3/2$, $\alpha_4 = 1/2$.

We once again recover $\alpha_2 = 0$ for each configuration. Hence, the leading term of the LBF is still $1/8 \log N$. The comparison of our results and the CFT prediction is represented in Figure 4.12b. The multiplicative and additive constants for the functions (2.19) are given by

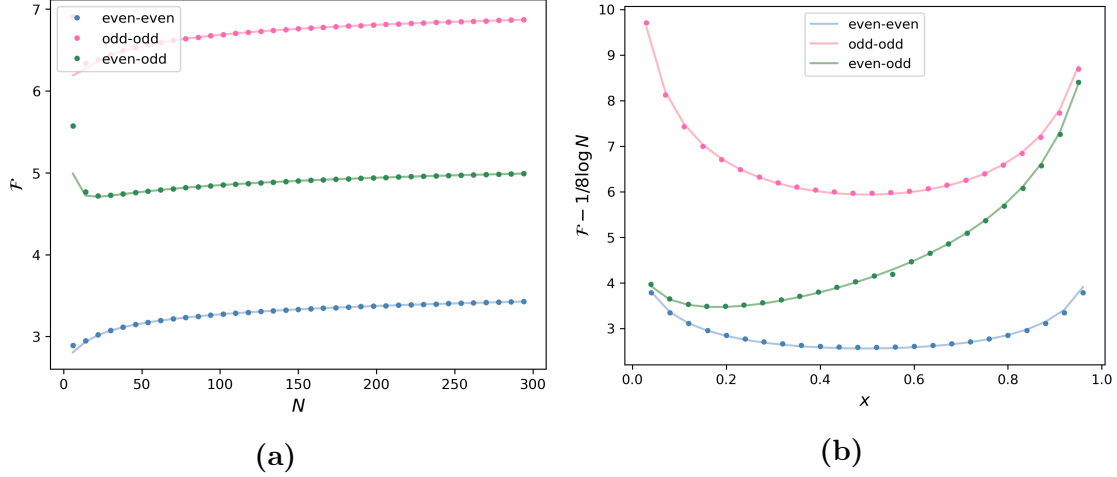


Figure 4.12: These figures show the results for Case 2. **(a)** The LBF as a function of N . The dotted and darker lines are our results and the continuous and lighter lines are the fits. **(b)** The subleading terms are a function of $x = N_A/N$ with $N = 100$ for the even cases and $N = 99$ for the odd ones. The dotted and darker lines are our results and the continuous and lighter lines are the CFT predictions.

- Even-even: $\xi_f = 0.0298 \pm 10^{-3}$, $\xi_g = 0.2062 \pm 10^{-1}$,
- Odd-odd: $\xi_f = -0.0406 \pm 10^{-2}$, $\xi_g = 0.1428 \pm 10^{-2}$,
- Even-odd: $\xi_f = 0.0327 \pm 10^{-2}$, $\xi_g = 0.3021 \pm 10^{-2}$.

As we see in Figure 4.12b, the behaviour of the subleading terms is different than in the previous cases but still follows the prediction (2.18).

4.4.5 Conclusion

In this section, we have studied the bipartite fidelity of the XX model with open boundary conditions. For this model, it is possible to write the bipartite fidelity as a determinant. For the special case $N_{A,B} = f$ with f even, it is possible to compute this determinant in closed form. For generic sizes, we compute the LBF numerically. Our results for both the leading and the subleading contributions are in excellent agreement with the known CFT predictions.

We then expanded the discussion to include the first excited state of the model. We considered two different combinations of ground states and first excited states. The bipartite fidelity is computed in the same way as in the ground state case. We find that for each configuration, the leading term of the LBF is still $1/8 \log N$. The subleading terms show differences compared to the ground state ones, but they still follow the CFT prediction. Many other configurations are possible. It would be interesting to study them to see if the leading term is always the same. In particular, one could consider the first excited state with a non-compact filling of fermions.

In Chapter 2, we have constructed a matrix that commutes with the reduction correlation matrix. The matrix $\mathcal{M}$ that appears in the study of the bipartite fidelity is similar to the correlation matrix as its elements are also expectation values of a

product of two operators. One may thus wonder if it would be possible to construct a matrix that commutes with this matrix $\mathcal{M}$. As the determinant of a matrix is the product of its eigenvalues, a commuting matrix would also be useful to find the eigenvalues.

Chapter 5

Krawtchouk chain

In this chapter, we construct an inhomogeneous model based on the Krawtchouk polynomials. This chain was first introduced in [31]. We first review some properties of the Krawtchouk polynomials. Then, we construct the chain using the formalism of Section 3.4. We study the entanglement entropy and the bipartite fidelity in the ground state.

5.1 Krawtchouk polynomials

It is convenient to introduce $L = N - 1$ in this section. The Krawtchouk polynomials, $\{K_n(x; L, p) \mid 0 < p < 1\}_{n=0}^L$, are a finite family of discrete orthogonal polynomial related to the binomial distribution. They are defined in terms of a hypergeometric function as [32]

$$K_n(x; L, p) = {}_2F_1 \left(\begin{matrix} -n, & -x \\ & -L \end{matrix}; \frac{1}{p} \right) = \sum_{k=0}^n \frac{(-n)_k (-x)_k}{(-L)_k} \frac{1}{p^k k!}. \quad (5.1)$$

To lighten the notations, we write $K_n(x) = K_n(x; L, p)$. From this definition, we see that the Krawtchouk polynomials are self-dual, $K_n(x) = K_x(n)$. The graphs of the first few polynomials are represented in Figure 5.1 and their expressions are

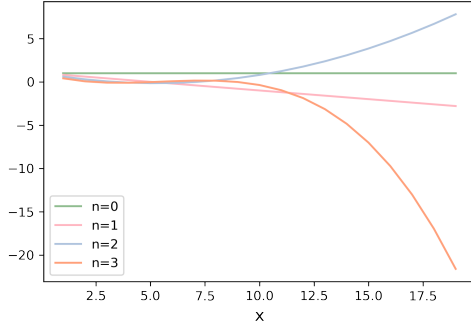
$$\begin{aligned} K_0(x) &= 1, \\ K_1(x) &= 1 - \frac{x}{Lp}, \\ K_2(x) &= 1 - x \left(\frac{2}{Lp} + \frac{1}{L(L-1)p^2} \right) + x^2 \frac{1}{L(L-1)p^2}. \end{aligned} \quad (5.2)$$

We now state and prove some properties of the Krawtchouk polynomials that will be useful in our work. We refer to [42] for a more complete overview of these polynomials.

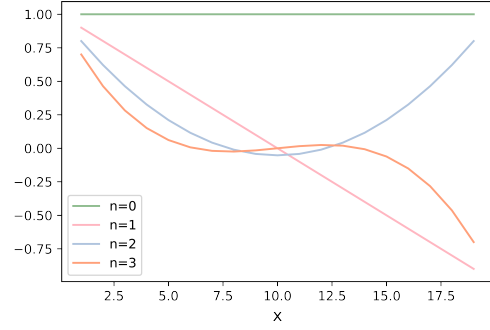
Proposition 5.1.1 (Generating function). *The generating function of the Krawtchouk polynomials is*

$$G(x, z) = \left(1 - \frac{1-p}{p} z \right)^x (1+z)^{L-x} = \sum_{n=0}^{\infty} \binom{L}{n} K_n(x) z^n, \quad (5.3)$$

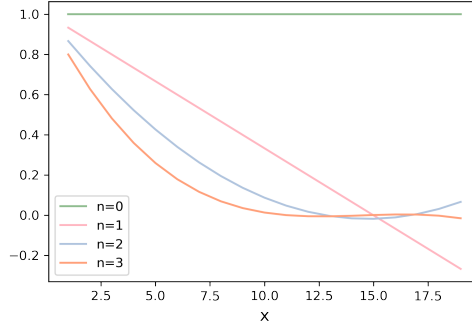
with the convention $\binom{L}{n} = 0$ when $n > L$.



(a) $p = 1/4$.



(b) $p = 1/2$.



(c) $p = 3/4$.

Figure 5.1: The Krawtchouk polynomials of degree $n = 0, \dots, 3$ for $L = 20$ and different values of p .

Proof. Let us start from the right-hand side. Using the definition of the Krawtchouk polynomials and writing the Pochhammer symbols in terms of factorials, we have

$$\begin{aligned}
 \sum_{n=0}^L \binom{L}{n} K_n(x) z^n &= \sum_{n=0}^L \sum_{k=0}^x \binom{L}{n} \frac{(-1)^k z^n}{p^k} \frac{n!(L-n)!}{L!} \frac{(L-k)!}{(n-k)!(L-n)!} \frac{x!}{k!(x-k)!} \\
 &= \sum_{k=0}^x \left[\sum_{n=0}^L \binom{L-k}{n-k} z^{n-k} \right] \binom{x}{k} \frac{(-1)^k z^k}{p^k} \\
 &= \sum_{k=0}^x \left[\sum_{n=0}^{L-k} \binom{L-k}{n} z^n \right] \binom{x}{k} \frac{(-1)^k z^k}{p^k}.
 \end{aligned} \tag{5.4}$$

The sum over n is the binomial expansion of $(1+z)^{L-k}$. Therefore, we have

$$\begin{aligned}
 \sum_{n=0}^L \binom{L}{n} K_n(x) z^n &= \sum_{k=0}^x (1+z)^{L-k} \binom{x}{k} \frac{(-1)^k z^k}{p^k} \\
 &= (1+z)^L \sum_{k=0}^x \binom{x}{k} \frac{(-1)^k z^k}{p^k} (1+z)^{-k}.
 \end{aligned} \tag{5.5}$$

The sum over k is the binomial expansion of $\left(1 - \frac{z}{(1+z)p}\right)^x$. After some rewrirting,

we obtain

$$\sum_{n=0}^L \binom{L}{n} K_n(x) z^n = (1+z)^{L-x} \left(1 - \frac{1-p}{p} z\right)^x, \quad (5.6)$$

which concludes the proof. $\square$

We note that, using Cauchy's integral formula [43] and the generating function, the Krawtchouk polynomials can be expressed as a contour integral:

$$K_n(x) = \frac{1}{\binom{L}{n}} \frac{1}{2\pi i} \oint_0 \left(1 - \left(\frac{1-p}{p}\right) z\right)^k (1+z)^{L-k} \frac{1}{z^{n+1}} dz. \quad (5.7)$$

Proposition 5.1.2 (Orthogonality). *The orthogonality relation for the Krawtchouk polynomials has the form (3.67) with*

$$w(x) = \binom{L}{x} p^x (1-p)^{L-x}, \quad v_n = \left(\frac{1-p}{p}\right)^n / \binom{L}{n}. \quad (5.8)$$

Proof. Let us define the sum

$$P(y, z) = \sum_{x=0}^L \binom{L}{x} p^x (1-p)^{L-x} \left[\sum_{n=0}^L \binom{L}{n} K_n(x) z^n \right] \left[\sum_{m=0}^L \binom{L}{m} K_m(x) y^m \right]. \quad (5.9)$$

Using the definition of the generating function of the Krawtchouk polynomials, we have that

$$\begin{aligned} P(y, z) &= \sum_{x=0}^L \binom{L}{x} p^x (1-p)^{L-x} \left(1 - \frac{1-p}{p} z\right)^x (1+z)^{L-x} \\ &\quad \times \left(1 - \frac{1-p}{p} y\right)^x (1+y)^{L-x}. \end{aligned} \quad (5.10)$$

This sum is a binomial expansion and thus can be expressed as

$$P(y, z) = \left(p \left(1 - \frac{1-p}{p} z\right) \left(1 - \frac{1-p}{p} y\right) + (1+p)(1+z)(1+y) \right)^L \quad (5.11)$$

After some algebra, we find

$$P(y, z) = \left(1 + \left(\frac{1-p}{p}\right) yz\right)^L = \sum_{n=0}^L \binom{L}{n} \left(\frac{1-p}{p}\right)^n z^n y^n. \quad (5.12)$$

Therefore, comparing this expression with (5.9), we find that if $n \neq m$,

$$\sum_{x=0}^L \binom{L}{x} p^x (1-p)^{L-x} K_n(x) K_m(x) = 0, \quad (5.13)$$

and if $n = m$,

$$\sum_{x=0}^L \binom{L}{x} p^x (1-p)^{L-x} K_n(x) K_n(x) = \left(\frac{1-p}{p}\right)^n / \binom{L}{n}, \quad (5.14)$$

which concludes the proof. $\square$

Proposition 5.1.3 (Recurrence). *The recurrence relation for the Krawtchouk polynomials is given by (3.68) with*

$$\lambda(x) = x, \quad A_n = -p(L - n), \quad C_n = -n(1 - p). \quad (5.15)$$

Proof. We use the generating function to prove the recurrence relation. Taking the derivative with respect to z of both sides of (5.3), we have

$$\begin{aligned} \sum_{n=0}^L n K_n(x) z^{n-1} &= -x \left(\frac{1-p}{p} \right) \left(1 - \left(\frac{1-p}{p} \right) z \right)^{x-1} (1+z)^{L-x} \\ &\quad + (L-x)(1+z)^{L-x-1} \left(1 - \left(\frac{1-p}{p} \right) z \right)^x. \end{aligned} \quad (5.16)$$

We multiply both sides of (5.16) by $\left(1 - \left(\frac{1-p}{p} \right) z \right) (1+z)$. The right-hand side gives

$$\begin{aligned} \text{RHS} &= \left(-x \left(\frac{1-p}{p} \right) (1+z) + (L-x) \left(1 - \left(\frac{1-p}{p} \right) z \right) \right) \\ &\quad \times \left(1 - \left(\frac{1-p}{p} \right) z \right)^x (1+z)^{L-x} \\ &= \left(\left(L - \frac{x}{p} \right) - L \left(\frac{1-p}{p} \right) z \right) \sum_{n=0}^L \binom{L}{n} K_n(x) z^n \\ &= \left(L - \frac{x}{p} \right) \sum_{n=1}^{L+1} \binom{L}{n-1} K_{n-1}(x) z^{n-1} \\ &\quad - L \left(\frac{1-p}{p} \right) \sum_{n=2}^{L+2} \binom{L}{n-1} K_{n-2}(x) z^{n-1}. \end{aligned} \quad (5.17)$$

The left-hand side is given by

$$\begin{aligned} \text{LHS} &= \left(1 - \left(\frac{1-p}{p} \right) z + z - \left(\frac{1-p}{p} \right) z^2 \right) \sum_{n=0}^L \binom{L}{n} n K_n(x) z^{n-1} \\ &= \sum_{n=0}^L \binom{L}{n} n K_n(x) z^{n-1} \left(1 - \left(\frac{1-p}{p} \right) z \right) \sum_{n=1}^{L+1} \binom{L}{n-1} (n-1) K_{n-1}(x) z^{n-1} \\ &\quad - \left(\frac{1-p}{p} \right) \sum_{n=2}^{L+2} \binom{L}{n-2} (n-2) K_{n-2}(x) z^{n-1}. \end{aligned} \quad (5.18)$$

In each sum, we take the $n+1$ -th terms, with $2 \leq n+1 \leq L$. Then, we have

$$\begin{aligned} &\binom{L}{n+1} (n+1) K_{n+1}(x) - \left(\binom{L}{n} n - \binom{L}{n} \left(\frac{1-p}{p} \right) n \right) K_n(x) \\ &\quad - \binom{L}{n-1} \left(\frac{1-p}{p} \right) (n-1) K_{n-1}(x) \\ &= \binom{L}{n} \left(L - \frac{x}{p} \right) K_n(x) - L \left(\frac{1-p}{p} \right) \binom{L}{n-1} K_{n-1}(x). \end{aligned} \quad (5.19)$$

After some algebra, we find

$$-xK_n(x) = p(L-n)K_{n+1}(x) - [p(L-n) + n(1-p)]K_n(x) + n(1-p)K_{n-1}(x), \quad (5.20)$$

which concludes the proof. $\square$

Proposition 5.1.4 (Difference). *The difference relation for the Krawtchouk polynomials is given by (3.69) with*

$$f(n) = n, \quad \bar{A}(x) = -p(L-x), \quad \bar{C}(x) = -x(1-p). \quad (5.21)$$

Proof. This relation follows from the self-duality of the Krawtchouk polynomials and the recurrence relation. $\square$

Proposition 5.1.5 (Symmetry). *The Krawtchouk polynomials satisfy the symmetry relation*

$$K_n(x; L, p) = (-1)^n \left(\frac{1-p}{p} \right)^n K_n(L-x; L, 1-p). \quad (5.22)$$

Proof. We prove this property by induction. Let us first note that the recurrence coefficients (5.15) are such that, indicating the dependence in p ,

$$A_n(1-p) = -(1-p)(L-n) = \frac{1-p}{p}A_n(p), \quad C_n(1-p) = -np = \frac{p}{1-p}C_n(p). \quad (5.23)$$

For the case $n = 0$, we have

$$K_0(x; L, p) = 1 = (-1)^0 \left(\frac{1-p}{p} \right)^0 K_0(L-x; L, 1-p). \quad (5.24)$$

Let us suppose that the property is satisfied for $K_n(x)$ and show it is also satisfied for $K_{n+1}(x)$. Using the recurrence relation, we have

$$\begin{aligned} K_{n+1}(L-x; L, 1-p) &= \frac{1}{A_n(1-p)} [(A_n(1-p) \\ &\quad + C_n(1-p) + L-x)K_n(L-x; L, 1-p) \\ &\quad - C_n(p)K_{n-1}(L-x; L, 1-p)] \\ &= \frac{p}{1-p} \frac{1}{A_n(p)} [(A_n(1-p) \\ &\quad + C_n(1-p) + L-x)(-1)^n \left(\frac{p}{1-p} \right)^n K_n(x; L, p) \\ &\quad - \frac{p}{1-p} C_n(p)(-1)^{n-1} \left(\frac{p}{1-p} \right)^{n-1} K_{n-1}(x; L, p)] \\ &= (-1)^{n+1} \left(\frac{p}{1-p} \right)^{n+1} \frac{1}{A_n(p)} [-(A_n(1-p) \\ &\quad + C_n(1-p) + L-x)K_n(x; L, p) \\ &\quad - C_n(p)K_{n-1}(x; L, p)]. \end{aligned} \quad (5.25)$$

The coefficients are such that

$$\begin{aligned}
-(A_n(1-p) + C_n(1-p) + L - x) &= (1-p)(L-n) + np - L + x \\
&= -p(L-n) - n(1-p) + x \\
&= A_n(p) + C_n(p) + x.
\end{aligned} \tag{5.26}$$

Thus, the polynomials satisfy

$$\begin{aligned}
K_{n+1}(L-x; L, 1-p) &= (-1)^{n+1} \left(\frac{p}{1-p} \right)^{n+1} \frac{1}{A_n(p)} [(A_n(p) + C_n(p) + x)K_n(x; L, p) \\
&\quad - C_n(p)K_{n-1}(x; L, p)] \\
&= (-1)^{n+1} \left(\frac{p}{1-p} \right)^{n+1} K_{n+1}(x; L, p),
\end{aligned} \tag{5.27}$$

which concludes the proof. $\square$

Proposition 5.1.6 (Derivative). *The derivative of $K_n(x)$ with respect to x is given by*

$$K'_n(x) = \frac{1}{\binom{L}{n}} \sum_{j=1}^n \frac{(-1)^{j+1}}{j} \left(\left(\frac{p-1}{p} \right)^j - 1 \right) \binom{L}{n-j} K_{n-j}(x). \tag{5.28}$$

Proof. We derive the generating function (5.3) with respect to x :

$$\frac{\partial G(x, z)}{\partial x} = \left(\log \left(1 - \frac{(1-p)}{p} z \right) - \log(1+z) \right) G(x, z) = \sum_{n=0}^{\infty} \binom{L}{n} K'_n(x) z^n. \tag{5.29}$$

We consider the series expansion of the logarithm to write the left-hand side of the expression as a product of two infinite sums

$$\left[\sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{m} \left(\left(\frac{p-1}{p} \right)^m - 1 \right) z^m \right] \left[\sum_{k=0}^{\infty} \binom{L}{k} K_k(x) z^k \right] = \sum_{k=0}^{\infty} \binom{L}{k} K'_k(x) z^k. \tag{5.30}$$

We use the Cauchy product formula to calculate the left-hand side. Then, we have

$$\sum_{k=0}^{\infty} \sum_{j=1}^k \frac{(-1)^{j+1}}{j} \left(\left(\frac{p-1}{p} \right)^j - 1 \right) \binom{L}{k-j} K_{k-j}(x) z^k = \sum_{k=0}^{\infty} \binom{L}{k} K'_k(x) z^k. \tag{5.31}$$

Taking the n -th term of the sums on both sides, we finally have

$$K'_n(x) = \frac{1}{\binom{L}{n}} \sum_{j=1}^n \frac{(-1)^{j+1}}{j} \left(\left(\frac{p-1}{p} \right)^j - 1 \right) \binom{L}{n-j} K_{n-j}(x), \tag{5.32}$$

which concludes the proof. $\square$

5.2 The model

To construct the model, we use the relations derived in Section 3.4. The parameters are then, choosing $\epsilon = +1$,

$$\begin{cases} J_n = \sqrt{p(1-p)(N-1-n)(n+1)}, \\ B_n = -((N-1)p + n(1-2p)). \end{cases} \quad (5.33)$$

Note that the magnetic field is constant if and only if $p = 1/2$ and its value is $B_n = -(N-1)/2$. We also have

$$\alpha_n = \alpha_0 \left(\frac{1-p}{p} \right)^{\frac{n}{2}} / \binom{N}{n}^{1/2}. \quad (5.34)$$

From the orthogonality relations (3.16), (3.67), we find that $\alpha_0 = 1$. The eigenfunctions are then given by, with $\omega_k = k$,

$$\phi_{n,k} = (-1)^n \left(\frac{p}{1-p} \right)^{n/2} \sqrt{\binom{N-1}{n} \binom{N-1}{k}} \sqrt{p^k(1-p)^{N-1-k}} K_n(k). \quad (5.35)$$

From the difference relation, we find

$$\lambda_n = n, \quad \bar{J}_k = -\sqrt{p(1-p)(N-1-k)(k+1)}, \quad \bar{B}_k = -[(N-1)p + k(1-2p)]. \quad (5.36)$$

The elements of the commuting matrix are given by

$$\begin{cases} t_n = 2(n-\ell+1)\sqrt{p(1-p)(N-1-n)(n+1)}, \\ d_n = [(N-1)p + n(1-2p)](2n-2\ell+1) - n(2f-1). \end{cases} \quad (5.37)$$

5.3 Entanglement entropy

We wish to study the model at half-filling. To achieve this, we add $-(N-1)/2$ to the magnetic field so that the eigenvalues are shifted and now given by $\omega_k = k - (N-1)/2$. Thus, ω_k takes negative values in the interval $[0, (N-1)/2]$. With this observation, we construct the ground state of the Krawtchouk chain.

If N is even, the ground state is simple and is a state with $f = N/2$ fermions. If N is odd, we have a zero eigenvalue when $k = (N-1)/2$. The ground state has a multiplicity of two for odd N and is a state with either $f = \lfloor N/2 \rfloor$ or $f = \lfloor N/2 \rfloor - 1$ fermions. The energy level of the ground state is then

$$E_0 = \sum_{k=0}^{f-1} \left(k - \frac{N-1}{2} \right) = \frac{f}{2}(f-N) \quad (5.38)$$

We consider the case $f = \lfloor N/2 \rfloor$. Using (3.34) and (5.35), the reduced correlation matrix is

$$\begin{aligned} C_{mn} &= (-1)^{n+m} \left(\frac{p}{1-p} \right)^{\frac{n+m}{2}} \sqrt{\binom{N-1}{n} \binom{N-1}{m}} \\ &\times \sum_{k=0}^{f-1} \binom{N-1}{k} p^k (1-p)^{N-1-k} K_n(k) K_m(k), \end{aligned} \quad (5.39)$$

with $m, n = 0, \dots, \ell - 1$. The sum can be evaluated using the Christoffel-Darboux formula (3.59). For $m \neq n$, we have

$$C_{nm} = (-1)^{n+m} \left(\frac{p}{1-p} \right)^{\frac{n+m}{2}} \sqrt{\binom{N-1}{n} \binom{N-1}{m} \binom{N-1}{f-1}} p^f (1-p)^{N-f} (N-f) \\ \times \frac{[K_{f-1}(n)K_f(m) - K_f(n)K_{f-1}(m)]}{n-m}. \quad (5.40)$$

For the case $n = m$ of the Christoffel-Darboux formula (3.59), we use the derivative of the Krawtchouk polynomials that we derived in (5.28). We obtain

$$C_{nn} = \left(\frac{p}{1-p} \right)^n \binom{N-1}{n} \binom{N-1}{f-1} p^f (1-p)^{N-f} (N-f) \\ \times [K'_{f-1}(n)K_f(n) - K'_f(n)K_{f-1}(n)]. \quad (5.41)$$

5.3.1 Numerical results

In this section, we compute the entanglement entropy numerically and compare our results with some known conjectures. We compute the entanglement in two different ways, as we did for the XX model. The first one is finding the eigenvalues from the correlation matrix directly from the correlation matrix defined in (5.39). The other one is with the help of the commuting matrix defined in (5.37) with $f = \lfloor N/2 \rfloor$. Once again, the two methods give the same results as expected. It is still not clear whether the commuting matrix has any advantages.

Numerical simulations involving the Krawtchouk polynomials face other issues. Indeed, as the length of the chain increases, we have to deal with higher degree polynomials. These computations lead to numerical instabilities as the precision of `python` cannot handle such objects well. We still conduct the simulations for systems up to $\ell = 20$ and $N = 60$.

We first look at the entanglement entropy as a function of ℓ for fixed N and different values of p . When $p = 1/2$, the magnetic field is constant. For this particular value of p and at half-filling, it is possible to use techniques from CFT in a curved background to find analytically the behaviour of the entropy. Finkel and González-López conjectured that the leading term of the entropy for $p = 1/2$ is given by [44]

$$S_\ell = \frac{1}{6} \log \left(2\ell \left(1 - \frac{\ell}{N} \right) \right) + a, \quad (5.42)$$

with a a constant that we find using a fit. The comparison of our numerical results and (5.42) is shown in Figure 5.2. An expression for the oscillations is also given in [44]. We do not take it into account in our simulations and focus on the leading behaviour. It is interesting to note that the same leading coefficient is $1/6$, as was the case for the XX model. However, the CFT techniques used in [44] are only valid for a constant magnetic field. For the Krawtchouk chain, this is only the case for $p = 1/2$.

We still study the entropy for different values of p numerically. In Figure 5.3, we show the behaviour of the entropy for different values of p , different values of N

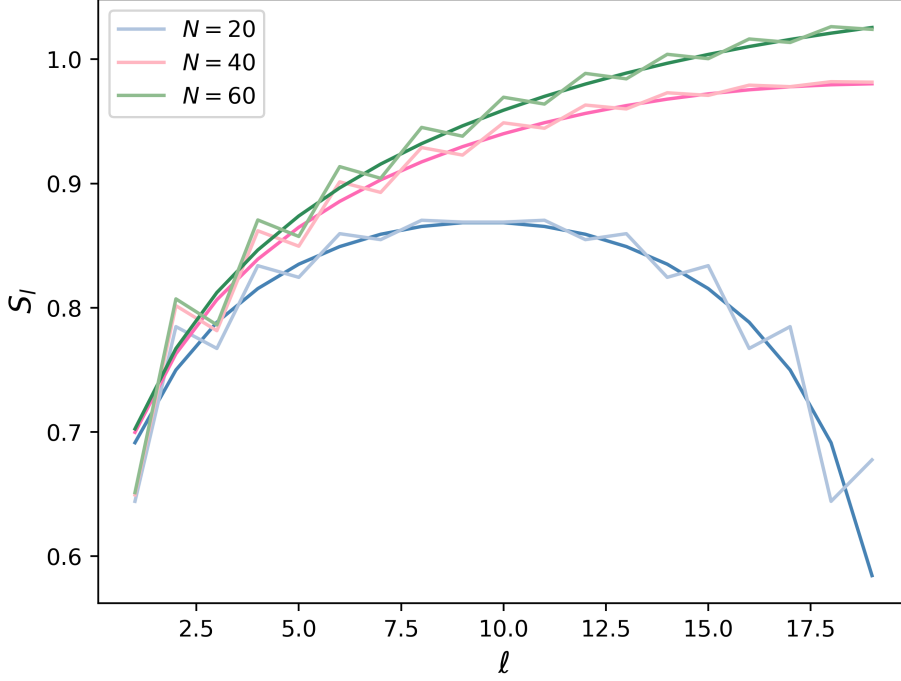


Figure 5.2: Entropy as a function of ℓ for $f = \lfloor N/2 \rfloor$ and different values of N . The lighter lines are our results and the darker ones are the conjecture. The additive constant is approximated numerically with a fit and is $a = 0.4769 \pm 10^{-3}$.

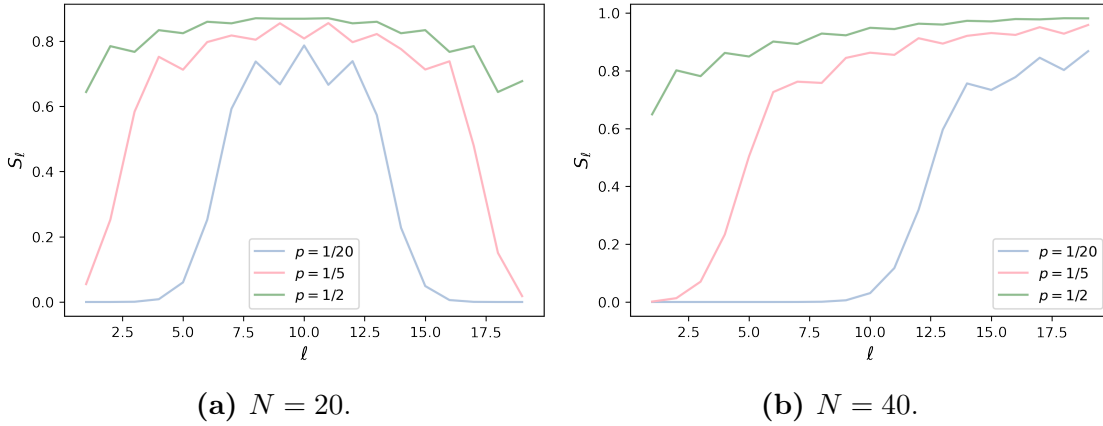


Figure 5.3: The entanglement entropy as a function of ℓ at half-filling. We consider different values of p and different values of N . When $p \neq 1/2$, we notice blocks where the entropy is close to zero in the beginning and the end of the chain. The size of these blocks increases as p goes to 0 or 1.

and subsystem lengths up to $\ell = 20$. We notice that for $p \neq 1/2$, the entropy is close to zero in some intervals $[0, \ell']$ and, by symmetry, $[N - \ell', N]$. We notice that the sizes of the intervals increase as p tends to either 0 or 1. Physically, this behaviour corresponds as a disentanglement of the spins localised in the ends from the rest of the chain. This indicates that some spins are in a product state and some form of order in the ground state of the system. We discuss this feature in more detail in Section 5.3.2.

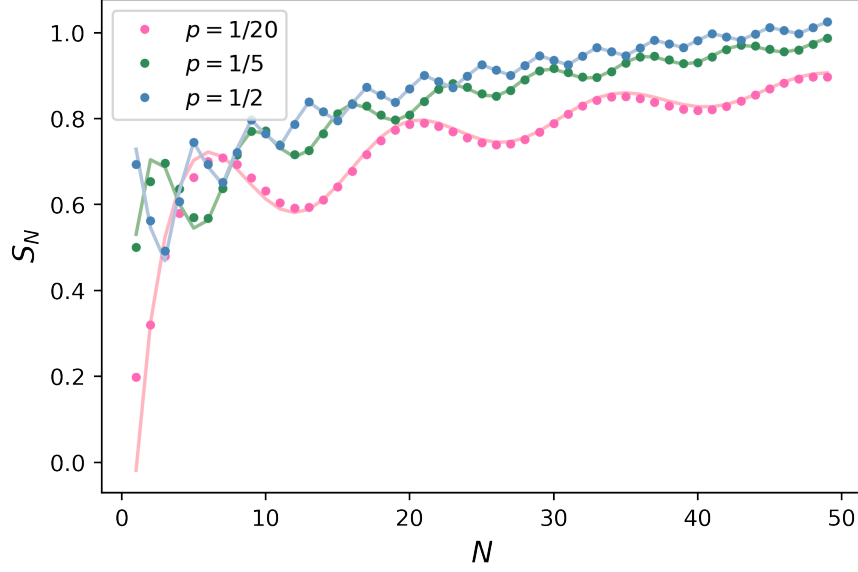


Figure 5.4: The entanglement entropy for the Krawtchouk chain as a function of N with $\ell = f = \lfloor N/2 \rfloor$ for a few values of p . The dotted and darker lines are our numerical results and the continuous and lighter lines are the conjecture (5.43).

Let us now analyse the entropy as a function of N for a fixed subsystem length $\ell = f = \lfloor N/2 \rfloor$. This corresponds to the maximal value of the entropy for each N . In Figure 5.4, we compute the entropy for different values of p and we see that the entropy also changes with p . Using numerical fits, Bernard et al. made a conjecture for the entropy as a function of N for $\ell = f = \lfloor N/2 \rfloor$ [45]

$$S_N = \frac{1}{6} \log \left(\frac{N}{2} \right) + a(p) - \frac{1}{2N} \frac{\cos \left(\frac{\pi}{2} \frac{N}{m(p)} \right)}{\sin \left(\frac{\pi}{2m(p)} \right)} + \dots, \quad (5.43)$$

with $a(p)$ a constant and

$$m(p) = \frac{1}{2} \left(1 - \log p + \frac{1 - \log 2}{2p} \right). \quad (5.44)$$

The comparison of the conjecture and our results is shown in Figure 5.4 for a few values of p . The additive constant can be computed using a fit. The results are represented in Figure 5.5. The leading term $1/6 \log(N/2)$ is valid for any p . The oscillations described by (5.43) are slightly off when p is close to 0 or 1. For these extreme values of p , the description of the oscillations can actually be refined to match the numerical results with more accuracy [46].

For the XX model, the correlation matrix has a special shape (Toeplitz+Hankel) and it is possible to compute an expression for the entropy analytically. For the Krawtchouk chain, the correlation matrix does not have any particular shape. It is thus not possible to use the same techniques. Finding analytically an expression for the entropy remains a challenge.

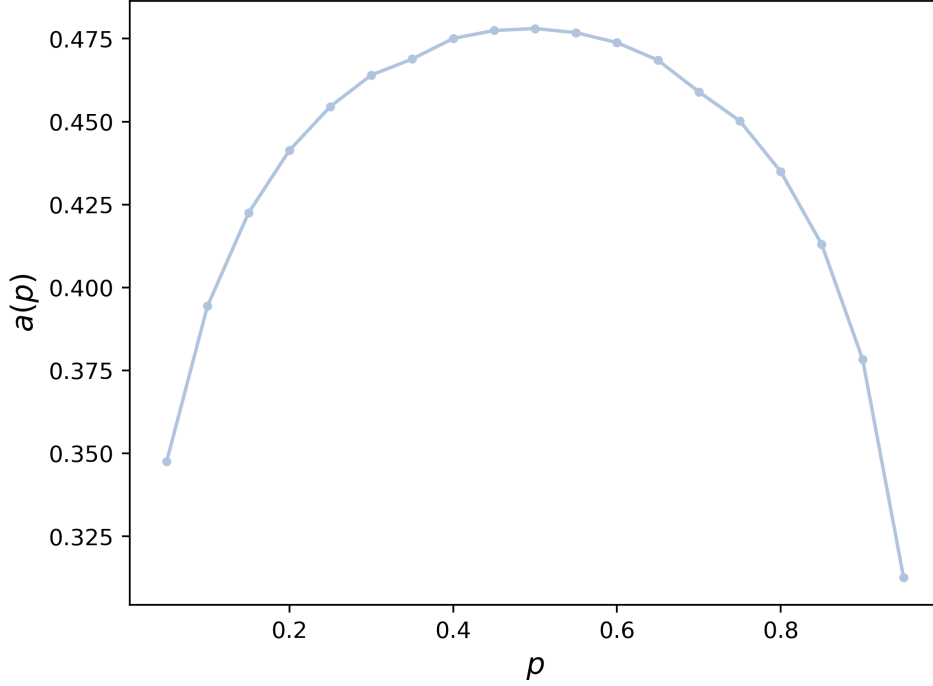


Figure 5.5: The additive constant $a(p)$ of the conjecture (5.43) as a function of p . The solid line is a guide for the eyes.

5.3.2 Local fermion density

As noticed in the previous section, when $p \neq 1/2$, the entropy vanishes in some intervals of the subsystem's length $[0, \ell']$ and $[N - \ell', N]$. Therefore, the spins localised in the beginning and in the end of the chain are not entangled with the rest of the chain. In other words, they are in a product state. This feature is one of the main differences between the XX and the Krawtchouk chains.

To investigate this property, we compute the so-called local fermion density. It is defined as the diagonal elements of the correlation matrix

$$\rho_n(p, f) = \langle c_n^\dagger c_n \rangle, \quad (5.45)$$

and is interpreted as the average number of fermions occupying the site n of the chain. For the Krawtchouk chain, we have

$$\rho_n(p, f) = \left(\frac{p}{1-p} \right)^n \binom{N-1}{n} \sum_{k=0}^{f-1} \binom{N-1}{k} p^k (1-p)^{N-1-k} K_n(k) K_n(k). \quad (5.46)$$

In Figure 5.6, we represent the local density as a function of $x = n/N$, for different values of p and at half-filling. As expected, we see that the case $p = 1/2$ does not show any particular order. For $p \neq 1/2$, the density is equal to either 1 or 0 in some intervals localised on the first and last sites of the chain. This indicates some order in the ground state as we know we certainly if those sites are occupied or unoccupied by a fermion.

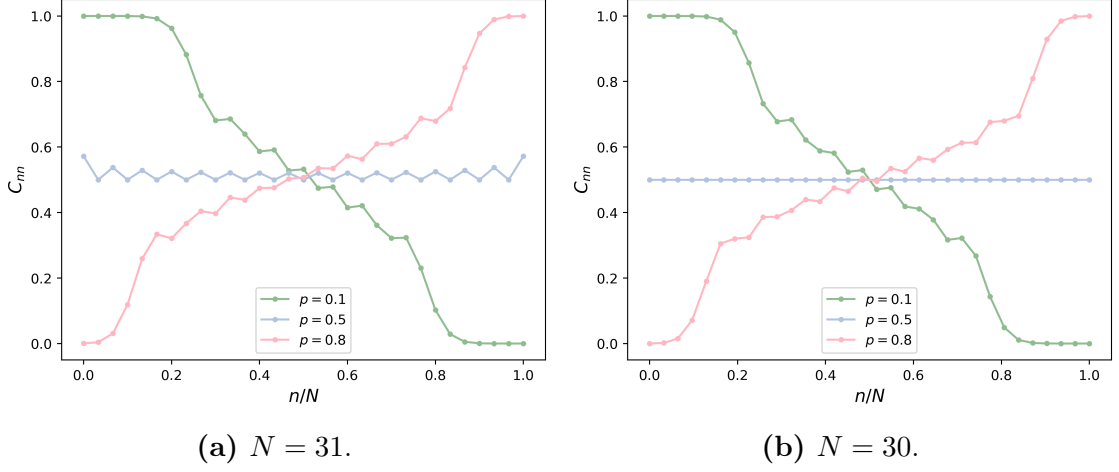


Figure 5.6: The local fermion density in the ground state for different values of p at half-filling.

We now derive some properties of the local fermion density.

Proposition 5.3.1 (Symmetry). *The local density (5.46) satisfy the symmetry relations*

$$\begin{aligned}
 (i) \quad & \rho_{N-1-n}(1-p, f) = \rho_n(p, f) \\
 (ii) \quad & \rho_{N-1-n}(p, N-f) = 1 - \rho_n(p, f)
 \end{aligned} \tag{5.47}$$

Proof. The proof of (i) directly follows from the symmetry property of the Krawtchouk polynomials (5.22). For (ii), we first complete the sum of (5.46) up to $k = N-1$,

$$\begin{aligned}
 \rho_{N-1-n}(p, N-f) &= \left(\frac{p}{1-p}\right)^{N-1-n} \binom{N-1}{n} \\
 &\times \left[\sum_{k=0}^{N-1} \binom{N-1}{k} p^k (1-p)^{N-1-k} K_{N-1-n}(k)^2 \right. \\
 &\left. - \sum_{k=N-f}^{N-1} \binom{N-1}{k} p^{N-1-k} (1-p)^k K_{N-1-n}(N-1-k)^2 \right].
 \end{aligned} \tag{5.48}$$

Using properties of the binomial coefficients, we have

$$\begin{aligned}
 \rho_{N-1-n}(p, N-f) &= \left(\frac{p}{1-p}\right)^{N-1-n} \binom{N-1}{n} \\
 &\times \left[\sum_{k=0}^{N-1} \binom{N-1}{k} p^k (1-p)^{N-1-k} K_{N-1-n}(k)^2 \right. \\
 &\left. - \sum_{k=0}^{f-1} \binom{N-1}{k} p^{N-1-k} (1-p)^k K_{N-1-n}(N-1-k)^2 \right].
 \end{aligned} \tag{5.49}$$

With the help of the symmetry property of the Krawtchouk polynomials (5.22), we find that the first sum is exactly the orthogonality relation (5.14) for $K_n(k, N-1, 1-p)$. This term is thus equal to one and the second sum is exactly equal to $\rho_n(p, f)$ which proves the case (ii). $\square$

Proposition 5.3.2. *At half-filling with N even, $N = 2f$, and for $p = 1/2$, the local density is*

$$\rho_n(p, f) = 1/2, \quad (5.50)$$

for all $n = 0, \dots, N - 1$.

Proof. For $N = 2f$ with N even and $p = 1/2$, the local density (5.46) becomes

$$\rho_n(p, f) = \binom{2f-1}{n} \sum_{k=0}^{f-1} \binom{2f-1}{k} \frac{1}{2^{2f-1}} K_n(k)^2. \quad (5.51)$$

We complete the sum up to $k = 2f - 1$,

$$\begin{aligned} \rho_n(p, f) &= \binom{2f-1}{n} \sum_{k=0}^{2f-1} \binom{2f-1}{k} \frac{1}{2^{2f-1}} K_n(k)^2 \\ &\quad - \binom{2f-1}{n} \sum_{k=f}^{2f-1} \binom{2f-1}{k} \frac{1}{2^{2f-1}} K_n(k)^2. \end{aligned} \quad (5.52)$$

The first sum is exactly the orthogonality relation for the Krawtchouk polynomials (5.14) and is thus equal to one. Using the properties of the binomial coefficients and the symmetry property of the Krawtchouk polynomials, the second term is exactly $\rho_n(p, f)$. Thus, we have

$$\rho_n(p, f) = 1 - \rho_n(p, f), \quad (5.53)$$

and the conclusion follows. $\square$

Proposition 5.3.3 (Integral representation). *The local fermion density has the integral representation*

$$\rho_n(p, f) = -(1 + \kappa) \oint_{\kappa} \oint_0 \frac{(1+w)^{N-1} (\kappa-w)^n (1+t)^n (t^f - w^f)}{(1+t)^{N+1} (1+w)^n (\kappa-t)^n w^f (t-w)} \frac{dt}{2\pi i} \frac{dw}{2\pi i}, \quad (5.54)$$

with

$$\kappa = \frac{p}{1-p}, \quad \bar{\kappa} = \frac{1-p}{p}. \quad (5.55)$$

Proof. We use the self-duality of the Krawtchouk polynomials to write (5.46) as

$$\rho_n(p, f) = \kappa^n \binom{N-1}{n} \sum_{k=0}^{f-1} \binom{N-1}{k} \kappa^k (1-p)^{N-1} K_n(k) K_k(n). \quad (5.56)$$

We then write the Krawtchouk polynomials in their respective integral representations (5.7). The two binomial coefficients and κ^n, κ^k cancel out, leaving us with

$$\rho_n(p, f) = \sum_{k=0}^{f-1} \oint_0 \oint_0 \frac{((1-p)(1+z)(1+w))^{N-1}}{z^{n+1} w^{k+1}} \left(\frac{\kappa-z}{1+z} \right)^k \left(\frac{\kappa-w}{1+w} \right)^n \frac{dz}{2\pi i} \frac{dw}{2\pi i}. \quad (5.57)$$

We make the change of variable

$$t = \frac{\kappa - z}{1 + z}. \quad (5.58)$$

The associated contour integral is now taken around κ . Therefore, we have

$$\rho_n(p, f) = -(1 + \kappa) \sum_{k=0}^{f-1} \oint_{\kappa} \oint_0 \frac{(1+w)^{N-1}(\kappa-w)^n(1+t)^n}{(1+t)^{N+1}(1+w)^n(\kappa-t)^n w} \frac{t^k}{w^k} \frac{dt}{2\pi i} \frac{dw}{2\pi i}. \quad (5.59)$$

The sum over k is a geometric sum and yields

$$\sum_{k=0}^{f-1} \frac{t^k}{w^k} = \frac{t^f - w^f}{w^f} \frac{w}{t - w}. \quad (5.60)$$

We finally have

$$\rho_n(p) = -(1 + \kappa) \oint_{\kappa} \oint_0 \frac{(1+w)^{N-1}(\kappa-w)^n(1+t)^n}{(1+t)^{N+1}(1+w)^n(\kappa-t)^n} \frac{(t^f - w^f)}{w^f(t - w)} \frac{dt}{2\pi i} \frac{dw}{2\pi i}, \quad (5.61)$$

which concludes the proof. $\square$

It remains a challenge to derive the asymptotic behaviour for $N \rightarrow \infty$ for the local fermion density starting from either (5.46) or (5.54).

5.3.3 Charlier polynomials

It is not easy to work with the limit $N \rightarrow \infty$ of the Krawtchouk polynomials [47, 48]. However, the problem gets easier if we consider a stricter limit. In this section, we investigate the Krawtchouk polynomials for $N \rightarrow \infty$ and $p = \lambda/N$ with $\lambda > 0$. This limit leads to another set of orthogonal polynomials, called the Charlier polynomials [32]

$$\lim_{N \rightarrow \infty} K_n(x, N, \lambda/N) = C_n(x, \lambda) = C_n(x). \quad (5.62)$$

We compute this limit for every quantity of interest of the Krawtchouk polynomials to find their expression for the Charlier polynomials. The orthogonality relation for the Charlier polynomials is given by

$$\sum_{x=0}^{\infty} \frac{\lambda^x}{x!} e^{-\lambda} C_n(x) C_m(x) = n! \lambda^{-n} \delta_{nm}. \quad (5.63)$$

These polynomials are thus related to the Poisson distribution. The recurrence relation is (3.68) with the coefficients

$$A_n = -\lambda, \quad C_n = -n. \quad (5.64)$$

The model is then described by the physical parameters

$$J_n = \sqrt{\lambda(n+1)}, \quad B_n = -(\lambda + n). \quad (5.65)$$

We find that the eigenfunctions are given by

$$\phi_{n,k} = (-1)^n \sqrt{\frac{\lambda^n}{n!} \frac{\lambda^k}{k!}} e^{-\lambda/2} C_n(k), \quad (5.66)$$

and the reduced correlation matrix is then

$$C_{mn} = (-1)^{n+m} \sqrt{\frac{\lambda^{n+m}}{n!m!}} \sum_{k=0}^{\infty} \frac{\lambda^k}{k!} e^{\lambda} C_n(k) C_m(k), \quad (5.67)$$

with $m, n = 0, \dots, \ell - 1$. We notice that the sum in (5.67) is exactly the orthogonality relation and the coefficient in front is the inverse of the square norm. Thus, the reduced correlation matrix is the identity matrix

$$C_{nm} = \delta_{nm}. \quad (5.68)$$

This implies that the eigenvalues of the matrix are all equal to one and therefore, the entropy vanishes. The ground state of the system described by the Charlier polynomials is a state where every site is occupied by a fermion, or equivalently, a system where all the spins are up. Note that if we consider the limit $N \rightarrow \infty$ with $p = 1 - \lambda/N$ of the Krawtchouk polynomials, the correlation matrix's elements are all zero. In that case, the ground state is the state with no fermions, or equivalently, with all the spins down.

5.3.4 Conclusion

The Krawtchouk chain is an example of an inhomogeneous spin chain. In this section, we studied the entanglement entropy in the ground state. Our investigations were mostly numerical, as the analytical analysis is quite demanding. However, we were also limited numerically. The Krawtchouk chain has some similarities with the XX model. For instance, the entropy for both systems exhibits parity oscillations and they have the same $1/6$ leading coefficient. We then compared our numerical results with some known conjectures and saw that both results matched. A particular feature of the Krawtchouk chain appears when we consider $p \neq 1/2$. Indeed, we discovered that the spins localised at the ends of the chain were disentangled from the rest of the chain. To understand this behaviour, we investigated the fermion density in the chain. We have seen that some order appears in the ground state of the chain.

A promising path would be to rigorously find an expression for the leading term of the fermion density. It could be computed using the asymptotic of the Krawtchouk polynomials [47, 48]. The leading term of the asymptotic expansion changes with the values of the parameters n, k, p [48]. There exists one particular interval of n/N that matches exactly the interval where the density is not equal to one or zero. With that observation, it seems that an expression for the behaviour of the density could be derived. However, we were not able to find it in the context of this work, but this path seems promising and is worth being investigated.

To ease the calculations, we considered a stricter limit to the Charlier polynomials and found that the ground state of that model was uncorrelated. Another interesting limit to investigate would be the limit that leads to the Hermite polynomials [32].

5.4 Bipartite fidelity

In this section, we investigate the bipartite fidelity of the Krawtchouk chain. Let us first recall some results that we have already derived in the previous sections, now using the usual notations for the bipartite fidelity. The whole system is again a chain of length N . The physical parameters of the system are

$$J_n^N = \sqrt{p(1-p)(N-1-n)(n+1)}, \quad B_n^N = -[(N-1)p + n(1-2p)]. \quad (5.69)$$

The ground state of the system is given by

$$|A \cup B\rangle = \prod_{k=0}^{f-1} d_k^\dagger |0\rangle, \quad (5.70)$$

with the fermionic operators defined by

$$\begin{aligned} d_k &= \sqrt{\binom{N-1}{k} p^k (1-p)^{N-1-k}} \sum_{n=0}^{N-1} (-1)^n \left(\frac{p}{1-p}\right)^{n/2} \sqrt{\binom{N-1}{n}} K_n(k, N-1) c_n, \\ d_k^\dagger &= \sqrt{\binom{N-1}{k} p^k (1-p)^{N-1-k}} \sum_{n=0}^{N-1} (-1)^n \left(\frac{p}{1-p}\right)^{n/2} \sqrt{\binom{N-1}{n}} K_n(k, N-1) c_n^\dagger. \end{aligned} \quad (5.71)$$

As before, we choose to work at half-filling, that is, with $f = \lfloor N/2 \rfloor$ and $\omega_k = k - (N-1)/2$.

5.4.1 Two subsystems

Let us now consider two subsystems A and B of length N_A and N_B , respectively, such that $N = N_A + N_B$. The study of the bipartite fidelity for the Krawtchouk chain is quite different than the one for the XX model. Indeed, we are now dealing with an inhomogeneous system. Hence, the coupling constants depend on the position of the sites. For the Krawtchouk chain, they also depend on the length of the chain. In the homogeneous case, we defined the two subsystems by simply switching off the interactions between the two subsystems. If we strictly follow this procedure here, the two subsystems would not be Krawtchouk chains. Thus, it would be difficult to diagonalise the Hamiltonian, or, at least, we would not be able to use the results we derived previously for the Krawtchouk chain.

We consider instead that each of the subsystems forms a Krawtchouk chain on its own. The bipartite fidelity would thus tell us how similar the ground state of a Krawtchouk chain of length N is to the ground state of two adjacent and independent Krawtchouk chains of lengths N_A and N_B . In Figure 5.7, we represent the coupling constants for the whole chain and for the subsystems.

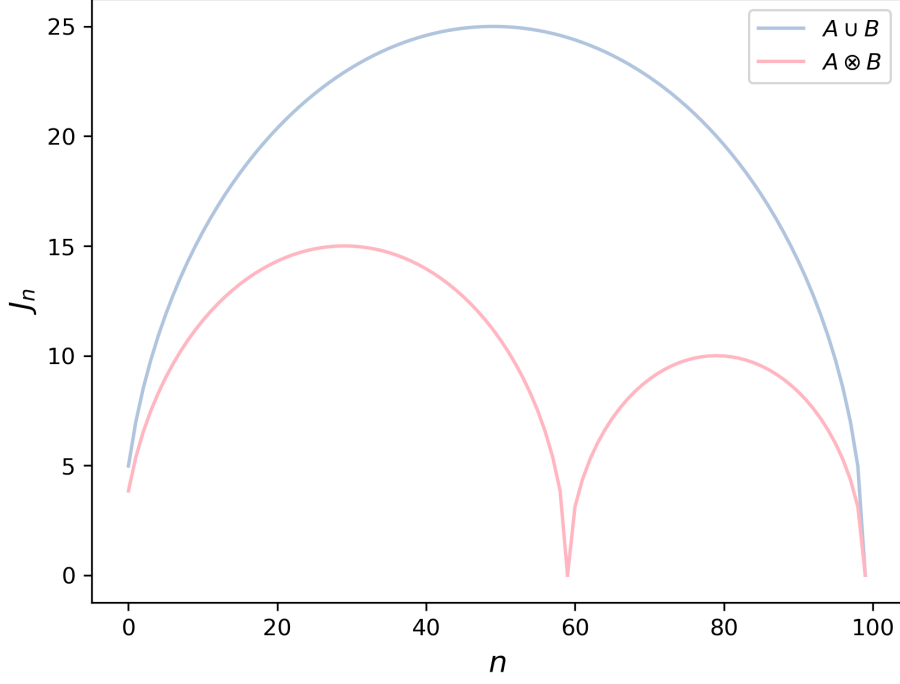


Figure 5.7: The coupling constants for the whole chain J_n^N and for the subsystems $J_n^{N_A}$, $J_n^{N_B}$ for $N = 100$, $N_A = 60$, $N_B = 40$ and $p = 1/2$.

The Hamiltonian of the two independent Krawtchouk chains is given by

$$\begin{aligned}
 \hat{H}_{A \otimes B} &= \underbrace{\sum_{n=0}^{N_A-2} J_n^{N_A} (c_n^\dagger c_{n+1} + c_n c_{n+1}^\dagger) - \sum_{n=0}^{N_A-1} B_n^{N_A} c_n^\dagger c_n}_{\hat{H}_A} \\
 &+ \underbrace{\sum_{n=N_A}^{N_B-2} J_{n-N_A}^{N_B} (c_n^\dagger c_{n+1} + c_n c_{n+1}^\dagger) - \sum_{n=N_A}^{N_B-1} B_{n-N_A}^{N_B} c_n^\dagger c_n}_{\hat{H}_B} \\
 &= \sum_{m,n=0}^{N-1} H_{mn} c_m^\dagger c_n.
 \end{aligned} \tag{5.72}$$

The matrix H is a $N \times N$ block diagonal matrix

$$H = \begin{pmatrix} H_A & 0 \\ 0 & H_B \end{pmatrix}, \tag{5.73}$$

where H_A (resp. H_B) is a $N_A \times N_A$ matrix (resp. $N_B \times N_B$) matrix associated to the subsystem A (resp. B). Both matrices can be diagonalised separately. Since both subsystems are Krawtchouk chains, the diagonalisation process is the same as for the whole system given in the previous section. Thus, the Hamiltonian is

$$\hat{H}_{A \otimes B} = \sum_{j=0}^{N-1} \gamma_j s_j^\dagger s_j, \tag{5.74}$$

and the fermionic operators are, for $0 \leq j \leq N_A - 1$,

$$s_j = \sqrt{\binom{N_A - 1}{j} p^j (1-p)^{N_A - 1 - j}} \sum_{n=0}^{N_A - 1} (-1)^n \left(\frac{p}{1-p}\right)^{n/2} \sqrt{\binom{N_A - 1}{n}} K_n(j, N_A - 1) c_n, \quad (5.75)$$

and, for $N_A \leq j \leq N - 1$,

$$s_j = \sqrt{\binom{N_B - 1}{j - N_A} p^{j - N_A} (1-p)^{N - 1 - j}} \times \sum_{n=0}^{N_B - 1} (-1)^n \left(\frac{p}{1-p}\right)^{n/2} \sqrt{\binom{N_B - 1}{n}} K_n(j - N_A, N_B - 1) c_{n + N_A}. \quad (5.76)$$

In both subsystems, we add a constant magnetic field to achieve half-filling in both parts. The eigenvalues γ_k are thus

$$\gamma_j = \begin{cases} j - \frac{N_A - 1}{2}, & 0 \leq j \leq N_A - 1, \\ j - N_A - \frac{N_B - 1}{2}, & N_A \leq j \leq N - 1. \end{cases} \quad (5.77)$$

The ground state is filled with f_A fermions in subsystem A and f_B fermions in subsystem B such that $f = f_A + f_B$. We write the ground state as

$$|A \otimes B\rangle = \prod_{i=0}^{f_A - 1} \prod_{j=N_A}^{N_A + f_B - 1} s_i^\dagger s_j^\dagger |0\rangle = \prod_{j=0}^{f-1} \tilde{s}_j^\dagger |0\rangle, \quad (5.78)$$

with

$$\tilde{s}_j = \begin{cases} s_j, & 0 \leq j \leq f_A - 1 \\ s_{N_A + j - f_A}, & f_A \leq j \leq f - 1. \end{cases} \quad (5.79)$$

If N_A and N_B are both even, the ground state is simple. Conversely, if both N_A and N_B are odd, the ground state has a multiplicity of four. If N_A and N_B have different parities, the ground state has a multiplicity of two.

5.4.2 Bipartite fidelity

To compute the bipartite fidelity, we take the scalar product of the ground states of the whole system and the subsystems

$$\mathcal{B} = |\langle A \otimes B | A \cup B \rangle|^2 = \left| \langle 0 | \prod_{j=0}^{f-1} \tilde{s}_{f-1-j} \prod_{k=0}^{f-1} d_k^\dagger | 0 \rangle \right|^2. \quad (5.80)$$

Since the fermionic operators are defined in terms of the $c_j, c_j^\dagger$ operators, we use Wick's theorem [28] to write the bipartite fidelity as a determinant

$$\mathcal{B} = \left| \det_{0 \leq j, k \leq f-1} \langle 0 | \tilde{s}_j d_k^\dagger | 0 \rangle \right|^2 = |\det \mathcal{M}|^2. \quad (5.81)$$

The matrix $\mathcal{M}$ is a $f \times f$ matrix. Its elements are defined as, for $0 \leq j \leq f_A - 1$,

$$\begin{aligned} \mathcal{M}_{jk} &= \sqrt{\binom{N_A-1}{j} \binom{N-1}{k}} p^{j+k} (1-p)^{N_A+N-j-k-2} \\ &\times \sum_{n=0}^{N_A-1} \left(\frac{p}{1-p}\right)^n \sqrt{\binom{N_A-1}{n} \binom{N-1}{n}} K_n(j, N_A-1) K_n(k, N-1), \end{aligned} \quad (5.82)$$

and, for $f_A \leq j \leq f-1$,

$$\begin{aligned} \mathcal{M}_{jk} &= (-1)^{N_A} \left(\frac{p}{1-p}\right)^{N_A/2} (p^{k+j-f_A} (1-p)^{N+N_B-j-k-2+f_A})^{1/2} \\ &\times \left(\binom{N_B-1}{j-f_A} \binom{N-1}{k} \right)^{1/2} \\ &\times \sum_{n=0}^{N_B-1} \left(\frac{p}{1-p}\right)^n \sqrt{\binom{N_B-1}{n} \binom{N-1}{n+N_A}} K_n(j-f_A, N_B-1) K_{n+N_A}(k, N-1) \end{aligned} \quad (5.83)$$

Numerical results

Finding a closed form for the determinant of the matrix $\mathcal{M}$ seems difficult, even for specific configurations as it was possible for the XX model. As the sums involve different Krawtchouk polynomials related to the different lengths, we cannot use the Christoffel-Darboux formula here. It is, however, possible to compute the LBF numerically. We follow the same procedure as in Section 4.4.3 for the XX model. We consider f even and the following configurations

- Even-even: $N = 2f$, $N_A = N_B = f$,
- Odd-odd: $N = 2f$, $N_A = f+1$, $N_B = f-1$,
- Even-odd: $N = 2f-1$, $N_A = f$, $N_B = f-1$.

We compute numerically the logarithmic bipartite fidelity $\mathcal{F} = -\log \mathcal{B}$ for $p = 1/2$. The results are represented in Figure 5.8. We fit these results using the same expression as the one used for the XX chain:

$$\mathcal{F}_{\text{fit}} = a_1 \log N + a_2 + a_3 \frac{\log N}{N} + a_4 \frac{1}{N}. \quad (5.84)$$

We find for each configuration

- Even-even: $a_1 = 0.09729 \pm 10^{-5}$, $a_2 = 0.02886 \pm 10^{-5}$,
 $a_3 = -0.0974 \pm 10^{-4}$, $a_4 = 0.03479 \pm 10^{-5}$,
- Odd-odd: $a_1 = 0.0940 \pm 10^{-4}$, $a_2 = 0.5274 \pm 10^{-4}$,
 $a_3 = -0.0234 \pm 10^{-3}$, $a_4 = 0.1606 \pm 10^{-4}$,
- Even-odd: $a_1 = 0.09687 \pm 10^{-5}$, $a_2 = 0.2302 \pm 10^{-3}$,
 $a_3 = -0.0196 \pm 10^{-3}$, $a_4 = 0.05493 \pm 10^{-5}$.

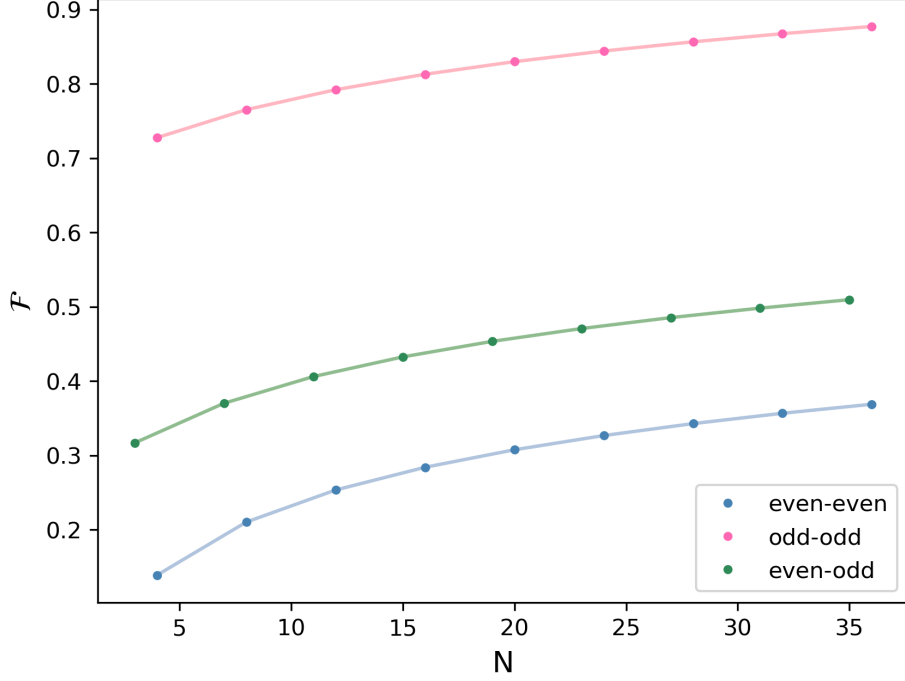


Figure 5.8: The logarithmic bipartite fidelity for the Krawtchouk chain for $p = 1/2$ for the different configurations. The dotted and darker lines are the numerical results and the continuous and lighter lines are the fits.

The a_1 term is $1/10$ up to a relative error of the order of 10^{-2} for the even-even and odd-odd configurations and of the order of 10^{-3} for the even-odd one. However, we were only able to compute the LBF numerically for subsystems up to $N = 40$ due to numerical instabilities. Thus, the value of the coefficients could change when considering larger systems. However, we expect the LBF to take higher values than for the XX model. The reason is that the coupling constants for the two subsystems are weaker than the ones for the whole Krawtchouk chain, as we can see in Figure 5.7. In particular, we are considering the chain cut in the middle and thus, the separation of the two subsystems is made when the coupling constant for the whole chain is near its maximum.

Let us now study the case of $p \neq 1/2$. Recall that for that choice of parameters, we observed a disentanglement of the spins localised at the ends of the chain. For the bipartite fidelity, this property has a lot of consequences. Indeed, if we consider $N_A = N_B = N/2$, the spins localised in the end of subsystem A and in the beginning of subsystem B are in the middle of the whole chain. Thus, in $A \otimes B$, we have uncorrelated spins localised in the beginning, in the middle and in the end of the chain. In the $A \cup B$ case, we only have uncorrelated spins in the beginning and the end.

The LBF is represented in Figure 5.9 for different values of p for the even-even configuration. We see in this figure that the behaviour of the LBF changes drastically as $p \neq 1/2$ and now diverges much faster. As the bipartite fidelity is a measure of similarity between the ground states of $A \otimes B$ and $A \cup B$, we explain this behaviour by the disentanglement of the spins, as explained earlier. The divergence is faster as p goes to 0 (or, similarly, to 1), which corresponds to the observation that the

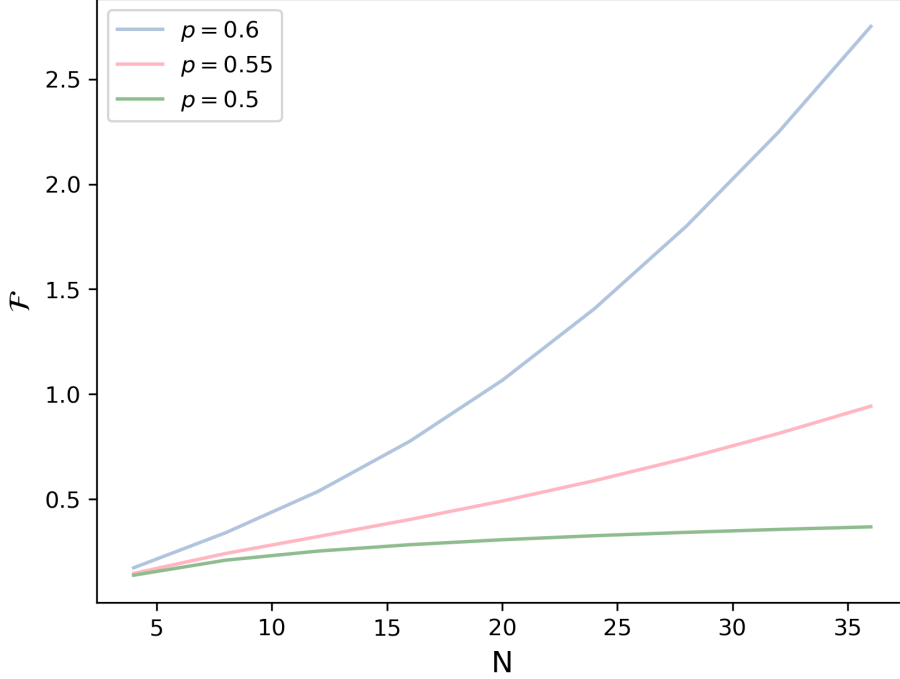


Figure 5.9: The logarithmic bipartite fidelity for the Krawtchouk chain for different values of p for the even-even configuration.

number of uncorrelated spins increases in this limit.

In Figure 5.10, we represent the LBF for $p = 1/4$ and for the different configurations. We try different functions to fit the LBF. The values of the coefficients for every case are given in the Appendix B. We see that the usual function for the bipartite fidelity (5.84) does not reproduce our results precisely, as we can see in Figure 5.10a. To understand this behaviour, we try different functions to fit the numerical data. We, however, always keep the $\log N$ term, as it is one of the main characteristics of the LBF. The cases shown in Figures 5.10d, 5.10e, and 5.10f match the data with more precision than (5.84). It seems that adding a N^2 term or N and $N \log N$ terms improves the accuracy of the fit.

This change in the behaviour of the LBF is another interesting characteristic of the Krawtchouk chain. The analytical analysis of the LBF is very demanding, and thus, confirming, denying, or refining our results is a real challenge. We could, however, already have a better understanding of the behaviour of the LBF with the numerical analysis of larger systems. The usual LBF function (5.84) could actually end up matching the data when considering large systems. If this is not the case, one may wonder if some physical phenomena are happening that would explain the change of behaviour when we go from $p = 1/2$ to $p \neq 1/2$.

5.4.3 Conclusion

In this section, we have studied the bipartite fidelity in the Krawtchouk chain. We used an adapted version of this quantity to be able to use all the results we derived in previous sections. We thus compared a Krawtchouk chain of length N to two

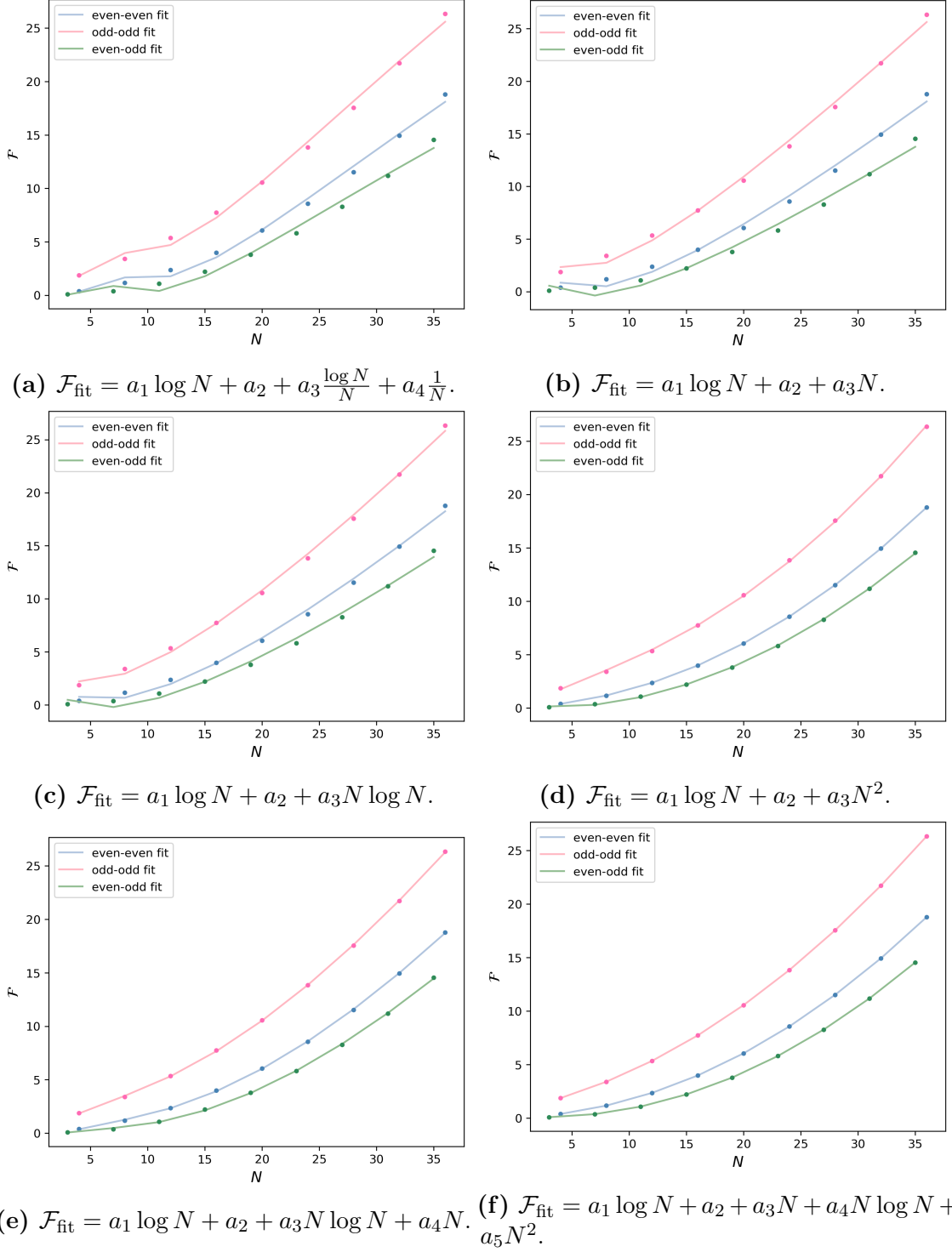


Figure 5.10: This figure shows the LBF for the Krawtchouk chain with $p = 1/4$ and different fits. The dotted and darker lines are our numerical results and the continuous and lighter lines are the numerical fits.

independent Krawtchouk chains of lengths N_A and N_B . As was the case for the XX chain, it is possible to write the bipartite fidelity as the determinant of a matrix. Because the entries of the matrix are here sums of a product of Krawtchouk polynomials, the analytical analysis of the LBF seems to be a real challenge. The numerical analysis is, however, possible but limited. For $p = 1/2$, we found that the

LBF had a logarithmic behaviour. The leading coefficient is close to $1/10$ but might change if we consider larger systems. The case $p \neq 1/2$ leads to a very different behaviour. Our numerical investigations seem to indicate the presence of another leading term. Once again, as we were limited to small systems, this conclusion could change. The first step for more accurate results would be to perform the numerical analysis for larger systems. Other programming languages than `python` should allow these investigations.

One may also wonder if the bipartite fidelity for the Krawtchouk chain also follows Stéphan and Dubail's prediction (2.18), or if a similar expression can be derived for inhomogeneous systems. To find out, one needs to calculate the Fermi velocity and the different conformal weights associated with each system. As the system is described by a CFT in curved spacetime, we might observe some changes.

It would also be interesting to compare the ground state of the XX model to the ground state of the Krawtchouk chain. It would help us understand the importance of the inhomogeneities in the chain by comparing them to a homogeneous system. It can be done by taking the scalar product of the two ground states. We end up with once again an expectation value of a product of operators, some related to the Krawtchouk chain and some to the XX chain. This expectation value can be written as a determinant by means of Wick's theorem. The matrix elements are sums of a product of Krawtchouk polynomials and a sine function. The numerical analysis is accessible, but it seems difficult to find a closed form for these sums analytically.

Chapter 6

Conclusion

In this thesis, we studied quantum entanglement in two one-dimensional systems. We used two different measures of entanglement, namely the entanglement entropy and the bipartite fidelity. The models we investigated are free-fermions models that we constructed from orthogonal polynomials. The first model we studied was the homogeneous XX model that rose up from the Chebyshev polynomials of the second kind. The second model is the inhomogeneous Krawtchouk chain constructed from the Krawtchouk polynomials.

For the XX chain, we studied the entropy in the ground state and the first excited state. For both states, the leading term of entropy has a logarithmic behaviour. In particular, in the limit of a large system, the entropy for the two states is the same and diverges as the logarithm of the subsystem's size. We also investigated the logarithmic bipartite fidelity for these two states. We saw that it diverges as the logarithm of the system's size. The behaviour is perfectly described by Dubail and Stéphan's CFT prediction.

We then studied the entanglement in the Krawtchouk chain. Some conjectures for the entropy are known, and we saw that our numerical results were in agreement with them. We noticed that for some values of the parameters p , the ground state of the Krawtchouk was partially in a product state. Indeed, we discovered that the spins localised in the beginning and end of the chain were disentangled from the rest of the chain. We then studied the bipartite fidelity for the Krawtchouk chain. We notice that the behaviour of the LBF drastically changes in the presence of disentangled spins. We tried to characterise this change numerically, and it seems like another leading term is present.

There are many open problems worth investigating in the future. The main ones are related to the analytical analysis of the Krawtchouk chain. An analytical proof for the leading term and the oscillations of the entropy (5.42),(5.43) is yet to be found. This problem is, however, expected to be very challenging as the reduced correlation matrix does not exhibit any particular shape. One could also investigate the entropy using CFT in a curved background, as done in [44], and try to extend the results to $p \neq 1/2$. It would also be interesting to provide an analytical proof for the behaviour of the local fermion density (5.46). This problem could be proven using the asymptotic expansion of the Krawtchouk polynomials. Lastly, the bipartite

fidelity for the Krawtchouk chain could also be investigated in more detail, especially for the case $p \neq 1/2$. A first step would be to conduct the numerical simulations for larger systems. It would allow us to have a better understanding of the behaviour of the bipartite fidelity. The analytical analysis seems, however, even more challenging than for the entropy as we now have to deal with different systems' lengths. One may also wonder if the bipartite fidelity could be studied with CFT, as was done for the entropy.

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Appendix A

Proofs

In this appendix, we present the proofs of two properties we encountered in chapter 2. Note that the notations used in this appendix are independent of the rest of the thesis. For instance, C is not the reduced correlation matrix defined in chapter 3

A.1 The Schmidt decomposition

Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be two Hilbert spaces of finite dimension $\dim \mathcal{H}_A = n_A$ and $\dim \mathcal{H}_B = n_B$. We define $m = \min(n_A, n_B)$. We consider two orthonormal bases of the Hilbert spaces $\{|e_i\rangle\}_{i=1}^{n_A} \subset \mathcal{H}_A$, $\{|f_i\rangle\}_{i=1}^{n_B} \subset \mathcal{H}_B$.

Any state $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ can be written as

$$|\psi\rangle = \sum_{j=1}^{n_A} \sum_{k=1}^{n_B} c_{jk} |e_j\rangle \otimes |f_k\rangle. \quad (\text{A.1})$$

The coefficients c_{jk} are the entries of a $n \times m$ matrix C . From the singular value theorem [27], one can find a unitary matrix $U = (u_{ij})_{i,j=1}^{n_A}$, a unitary matrix $V = (v_{ij})_{i,j=1}^{n_B}$ and a positive diagonal matrix $P = (p_{ij})_{i=0}^m$ such that

$$C = U \begin{pmatrix} P \\ 0 \end{pmatrix} V^\dagger. \quad (\text{A.2})$$

Therefore, the coefficients are

$$c_{jk} = \sum_{n,m=1}^r u_{jn} p_{nm} v_{km}^* = \sum_{n=1}^r p_{nn} u_{jn} v_{kn}^*. \quad (\text{A.3})$$

Moreover, we define

$$|\psi_n\rangle = \sum_{j=1}^{n_A} u_{jn} |e_j\rangle, \quad |\phi_n\rangle = \sum_{k=1}^{n_B} v_{kn}^* |f_k\rangle. \quad (\text{A.4})$$

These vectors form an orthonormal set of $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively,

$$\begin{aligned} \langle \psi_m | \psi_n \rangle &= \sum_{j,k=1}^{n_A} u_{km}^* u_{jn} \langle e_k | e_j \rangle = \sum_{j=1}^{n_A} u_{jm}^* u_{jn} = (U^\dagger U)_{mn} = \delta_{mn}, \\ \langle \phi_m | \phi_n \rangle &= \sum_{j,k=1}^{n_B} v_{km} v_{jn}^* \langle e_k | e_j \rangle = \sum_{j=1}^{n_B} v_{jm} v_{jn}^* = (V V^\dagger)_{mn} = \delta_{mn}. \end{aligned} \quad (\text{A.5})$$

Hence, the state $|\psi\rangle$ is decomposed as

$$|\psi\rangle = \sum_{n=1}^m p_{nn} |\psi_n\rangle \otimes |\phi_n\rangle. \quad (\text{A.6})$$

If we consider only the non-zero p_{nn} , the sum terminates at $\chi \leq m$.

A.2 Additivity of the entanglement entropy

We consider a bipartite system with Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ with $\dim \mathcal{H}_A = n_A$ and $\dim \mathcal{H}_B = n_B$. We consider two orthonormal bases of the Hilbert spaces for the subsystems: $\{|\psi_i^A\rangle\}_{i=1}^{n_A} \subset \mathcal{H}_A$ and $\{|\psi_j^B\rangle\}_{j=1}^{n_B} \subset \mathcal{H}_B$. We choose an orthonormal basis of $\mathcal{H}$ constructed as a tensor product: $\{|\psi_{ij}\rangle = |\psi_i^A\rangle \otimes |\psi_j^B\rangle \mid i = 1, \dots, n_A, j = 1, \dots, n_B\}$.

The density matrix of the system is a tensor product $\rho = \rho_A \otimes \rho_B$ with ρ_A (resp. ρ_B) the density matrix of subsystem A (resp. B). We denote by α_i^A and α_j^B the eigenvalues of the density matrices ρ_A and ρ_B , respectively. We thus have

$$\rho_A |\psi_i^A\rangle = \alpha_i^A |\psi_i^A\rangle, \quad \rho_B |\psi_j^B\rangle = \alpha_j^B |\psi_j^B\rangle. \quad (\text{A.7})$$

Therefore, the density matrix of the whole system satisfies the following equation:

$$\rho |\psi_{ij}\rangle = (\rho_A \otimes \rho_B) (|\psi_i^A\rangle \otimes |\psi_j^B\rangle) = \alpha_i^A \alpha_j^B |\psi_{ij}\rangle. \quad (\text{A.8})$$

With the definition of the logarithm of a matrix (2.10), we also have

$$\begin{aligned} \log \rho |\psi_{ij}\rangle &= \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} (\rho_A \otimes \rho_B - 1)^n |\psi_{ij}\rangle \\ &= \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} (\alpha_i^A \alpha_j^B - 1)^n |\psi_{ij}\rangle \\ &= \log (\alpha_i^A \alpha_j^B) |\psi_{ij}\rangle \\ &= (\log \alpha_i^A + \log \alpha_j^B) |\psi_{ij}\rangle. \end{aligned} \quad (\text{A.9})$$

Recall that the entropy is given by

$$\begin{aligned} S(\rho) &= -\text{Tr}(\rho \log \rho) \\ &= -\sum_{i=1}^{n_A} \sum_{j=1}^{n_B} \langle \psi_{ij} | \rho \log \rho | \psi_{ij} \rangle. \end{aligned} \quad (\text{A.10})$$

Making use of the orthonormality, $\langle \psi_{ij} | \psi_{kl} \rangle = \delta_{ik} \delta_{jk}$, and of the completeness relation, $\mathbb{I} = \sum_{i=1}^{n_A} \sum_{j=1}^{n_B} |\psi_{ij}\rangle \langle \psi_{ij}|$, we find that

$$\begin{aligned} S(\rho) &= -\sum_{i,k=1}^{n_A} \sum_{j,l=1}^{n_B} \langle \psi_{ij} | \rho | \psi_{kl} \rangle \langle \psi_{kl} | \log \rho | \psi_{ij} \rangle \\ &= -\sum_{i=1}^{n_A} \sum_{j=1}^{n_B} \alpha_i^A \alpha_j^B \log(\alpha_i^A \alpha_j^B) \\ &= -\sum_{j=1}^{n_B} \alpha_j^B \sum_{i=1}^{n_A} \alpha_i^A \log \alpha_i^A - \sum_{i=1}^{n_A} \alpha_i^A \sum_{j=1}^{n_B} \alpha_j^B \log \alpha_j^B. \end{aligned} \quad (\text{A.11})$$

Since the trace of a density matrix is one (2.6), we have $\sum_{i=1}^{n_A} \alpha_i^A = \sum_{j=1}^{n_B} \alpha_j^B = 1$. The entropy is then decomposed as

$$S(\rho) = - \sum_{i=1}^{n_A} \alpha_i^A \log \alpha_i^A - \sum_{j=1}^{n_B} \alpha_j^B \log \alpha_j^B = S(\rho_A) + S(\rho_B). \quad (\text{A.12})$$

Appendix B

Numerical data

This appendix contains the numerical results for the fits used for the LBF of the Krawtchouk polynomials for $p = 1/4$. They are represented in Figure 5.10.

(a) $\mathcal{F}_{\text{fit}} = a_1 \log N + a_2 + a_3 \frac{\log N}{N} + a_4 \frac{1}{N}$

- Even-even: $a_1 = 57.8901 \pm 10^0$, $a_2 = -232.9024 \pm 10^1$,
 $a_3 = 435.0399 \pm 10^1$, $a_4 = 8.8377 \pm 10^1$,
- Odd-odd: $a_1 = 68.70431 \pm 10^0$, $a_2 = -270.7006 \pm 10^1$,
 $a_3 = 497.9511 \pm 10^1$, $a_4 = 18.7613 \pm 10^1$,
- Even-odd: $a_1 = 43.2366 \pm 10^0$, $a_2 = -170.4854 \pm 10^2$,
 $a_3 = 284.8910 \pm 10^1$, $a_4 = 56.1116 \pm 10^0$.

(b) $\mathcal{F}_{\text{fit}} = a_1 \log N + a_2 + a_3 N$

- Even-even: $a_1 = -5.9639 \pm 10^{-1}$, $a_2 = 5.3207 \pm 10^0$,
 $a_3 = 0.9481 \pm 10^{-2}$,
- Odd-odd: $a_1 = -5.9861 \pm 10^{-1}$, $a_2 = 6.0704 \pm 10^0$,
 $a_3 = 1.1393 \pm 10^{-2}$,
- Even-odd: $a_1 = -4.7838 \pm 10^{-1}$, $a_2 = 3.4699 \pm 10^0$,
 $a_3 = 0.7802 \pm 10^{-3}$,

(c) $\mathcal{F}_{\text{fit}} = a_1 \log N + a_2 + a_3 N \log N$

- Even-even: $a_1 = -3.3425 \pm 10^{-1}$, $a_2 = 4.2745 \pm 10^0$,
 $a_3 = 0.2011 \pm 10^{-2}$,
- Odd-odd: $a_1 = -2.8225 \pm 10^{-1}$, $a_2 = 4.7908 \pm 10^0$,
 $a_3 = 0.2415 \pm 10^{-3}$,
- Even-odd: $a_1 = -2.8671 \pm 10^{-1}$, $a_2 = 3.0678 \pm 10^0$,
 $a_3 = 0.1693 \pm 10^{-2}$,

(d) $\mathcal{F}_{\text{fit}} = a_1 \log N + a_2 + a_3 N^2$

- Even-even: $a_1 = 0.1544 \pm 10^{-3}$, $a_2 = -0.0517 \pm 10^{-3}$,
 $a_3 = 0.014113 \pm 10^{-6}$,
- Odd-odd: $a_1 = 1.4065 \pm 10^{-1}$, $a_2 = -0.4613 \pm 10^{-1}$,
 $a_3 = 0.01688 \pm 10^{-4}$,
- Even-odd: $a_1 = -0.4189 \pm 10^{-2}$, $a_2 = 0.4951 \pm 10^{-1}$,
 $a_3 = 0.01263 \pm 10^{-5}$,

(e) $\mathcal{F}_{\text{fit}} = a_1 \log N + a_2 + a_3 N \log N + a_4 N$

- Even-even: $a_1 = 5.7908 \pm 10^{-1}$, $a_2 = 0.34 \pm 10^{-1}$,
 $a_3 = 0.8805 \pm 10^{-2}$, $a_4 = -3.2213 \pm 10^{-1}$,
- Odd-odd: $a_1 = 5.7777 \pm 10^{-1}$, $a_2 = 1.0859 \pm 10^{-1}$,
 $a_3 = 0.8812 \pm 10^{-2}$, $a_4 = -3.0333 \pm 10^{-1}$,
- Even-odd: $a_1 = 4.5737 \pm 10^{-1}$, $a_2 = 1.1921 \pm 10^{-1}$,
 $a_3 = 0.8001 \pm 10^{-2}$, $a_4 = -2.9298 \pm 10^{-1}$.

(f) $\mathcal{F}_{\text{fit}} = a_1 \log N + a_2 + a_3 N + a_4 N \log N + a_5 N^2$

- Even-even: $a_1 = 0.0665 \pm 10^{-3}$, $a_2 = -0.0318 \pm 10^{-4}$,
 $a_3 = 0.01421 \pm 10^{-5}$, $a_4 = -0.0095 \pm 10^{-4}$,
 $a_5 = 0.0390 \pm 10^{-3}$,
- Odd-odd: $a_1 = 0.075 \pm 10^{-3}$, $a_2 = 0.71551 \pm 10^{-4}$,
 $a_3 = 0.014155 \pm 10^{-6}$, $a_4 = -0.0055 \pm 10^{-4}$,
 $a_5 = 0.2147 \pm 10^{-4}$,
- Even-odd: $a_1 = -0.0161 \pm 10^{-3}$, $a_2 = 0.1019 \pm 10^{-3}$,
 $a_3 = 0.01433 \pm 10^{-5}$, $a_4 = -0.0188 \pm 10^{-3}$,
 $a_5 = -0.0202 \pm 10^{-3}$,

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