Towards the characterization of correlation functions and entanglement entropy in macroscopically excited states of the XY model

A DISSERTATION PRESENTED
BY
MARIO HENAO-AYALA.
TO
THE PHYSICS DEPARTMENT

IN PARTIAL FULFILLMENT OF THE REQUIREMENTS
FOR THE DEGREE OF
MASTER IN SCIENCE
IN THE SUBJECT OF
PHYSICS

UNIVERSIDAD DE LOS ANDES
BOGOTÁ, COLOMBIA
NOVEMBER 2018

2

Thesis advisor: Alonso Botero   Mario Henao-Ayala.

Towards the characterization of correlation functions and entanglement entropy in macroscopically excited states of the XY model

Abstract

In 2015 Brandão and Horodecki showed that for 1-dimensional quantum states the exponential decay of correlations implies area-law in their entanglement entropy. For practical reasons, physicists have studied mostly states that are usually much simpler than generic quantum states (e.g. the ground state); these states show an exponential decay in their correlation functions and consequently an area-law scaling of the entanglement entropy. On the other hand, *canonical typicality* tells us that the reduced density matrices of the overwhelming majority of the states of a quantum system correspond to canonical density matrices (tracing out the degrees of freedom of the environment) assuming a certain restriction on the total Hilbert space, resulting in volume-law scaling of entanglement entropy. If the particular restriction is that the total energy is constant, the canonical density matrices are thermal states.

In the full system, thermal states are mixtures of pure states and it is well known that they have exponential decay of correlations. However, from typicality arguments it is statistically very likely that each pure state constituting the thermal state follows volume-law scaling in its entropy of entanglement, hence it can not have exponential decay of correlations. In other words, at long distances, the fluctuations on the correlation functions due to the contribution of each pure state must cancel between them so the resulting signal for thermal states exhibits an exponentially decaying form.

In this work, we study the spatial mode structure of entanglement i.e. the relation between the depth of the modes, their frequency and their contribution to entanglement, for both the ground state and macroscopically excited states (eigenstates of the Hamiltonian describing a definite number of quasi-particle excitations) of the 1-dimensional XY model. We apply a principal component analysis to a *Gibbs sample* of fermionic covariance matrices of macroscopically excited states and study the fluctuations around the *mean* covariance matrix to under-

Thesis advisor: Alonso Botero   Mario Henao-Ayala.

stand the apparent paradox stated before between thermal states and
its constituents.

Resumen

En el año 2015 Brandão y Horodecki mostraron que para estados cuán-
ticos 1-dimensionales el decaimiento exponencial de las funciones de
correlación implica *leyes de area* en su entropía de enredamiento. Por
razones prácticas, los físicos han estudiado mayormente estados que
usualmente son mucho más simples que los estados cuánticos genéricos
(por ejemplo el estado base); éstos presentan un decaimiento exponen-
cial en sus funciones de correlación y como consecuencia *leyes de area*
en el escalamiento de la entropía de enredamiento. Por otro lado, la
tipicidad canónica dice que las matrices de densidad reducida de la
gran mayoría de estados de un sistema cuántico corresponden a matri-
ces densidad canónicas (traza parcial sobre los grados de libertad del
ambiente) asumiendo una cierta restricción del espacio de Hilbert total;
estos estados siguen *leyes de volumen* en su entropía de enredamiento.
Si la restricción es que la energía es constante las matrices densidad
canónicas son estados térmicos.

En el sistema total, los estados térmicos son una mezcla de estados
puros y se sabe bien que tienen correlaciones que decaen exponencial-
mente. Sin embargo, por argumentos de tipicidad es estadísticamente
muy probable que cada estado puro que constituye el estado térmico
sigue una *ley de volumen* en su entropía de enredamiento, lo que indica
que no puede tener correlaciones que decaen exponencialmente. En
otras palabras, para distancias largas las fluctuaciones en las funciones
de correlación debidas a las contribuciones de cada estado puro se deben
cancelar entre sí para que la señal resultante del estado térmico muestre
un comportamiento exponencial decayente.

En este trabajo, se estudia la estructura espacial del enredamiento,
es decir, la relación entre la profundidad de los modos, su frecuen-
cia y su contribución al enredamiento para el estado base y estados
macroscópicamente excitados (estados propios del Hamiltoniano que
representan un número definido de excitaciones de cuasi-partículas) del
modelo XY 1-dimensional. Se aplica un *principal component analysis*
a un muestreo de Gibbs de matrices de covarianza fermiónicas de es-
tados macroscópicamente excitados para estudiar las fluctuaciones al

Thesis advisor: Alonso Botero   Mario Henao-Ayala.

rededor de la matriz de covarianza media para entender la aparente paradoja mencionada anteriormente entre los estados térmicos y sus constituyentes.

Contents

List of figures

A mi familia. VON.

Acknowledgments

Quiero agradecer a todas las personas que me apoyan y creen en mí. En particular agradezco a mi familia, mis amigos y al Prof. Alonso Botero por su acompañamiento y enseñanzas.

1
Introduction

In quantum many-body systems on a lattice, entanglement is a property widely investigated since it provides information about certain universal properties of physical interest such as phase transitions [1–3]. Additionally, entanglement has applications in diverse quantum computation protocols [3–5].

Generic quantum states of a many-body system, that is, random pure states drawn from the Haar measure, give rise to sub-systems that are very nearly maximally correlated with their complementary sub-system. However, the most studied states in physics, the ground state, correspond to states much less entangled than they could be. There is enough evidence showing that entanglement measures, in a certain way, store information about the behavior of conventional correlation
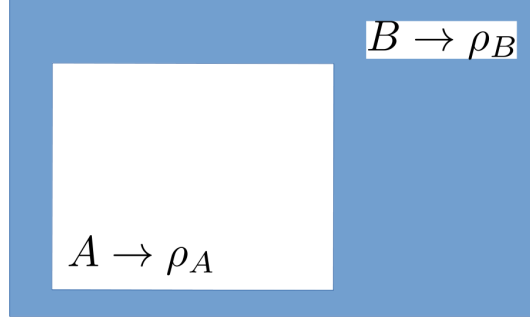
Figure 1.0.1: A partition of a system into two parts A and B.

functions. On the other hand, the study of correlation functions play a very important role in understanding the collective behavior of a system. A general way to quantify correlations between two regions A and B of a system is with the correlation function:

$$\mathrm{Cor}(A, B) := \max_{\|O_A\|\leq 1, \|O_B\|\leq 1} |\mathrm{tr}\{(O_A \otimes O_B)(\rho_{AB} - \rho_A \otimes \rho_B)\}|, \quad (1.1)$$

where O_A and O_B are operators acting in the sub-spaces A and B respectively and ρ_{AB}, ρ_A and ρ_B are the density matrices of the full system, the sub-system A and the sub-system B, respectively. We say that a system has exponential decay of correlations if

$$\mathrm{Cor}(A, B) \leq e^{-\frac{R}{\xi}} \quad (1.2)$$

for any A and B sub-regions of the system [further details in [6–8, 8]]. Here R is the separation (lattice distance) between the region and ξ is the correlation length.

It is natural to think that correlations between sub-systems must give some insights about the nature of entanglement between them; this is the reason there are several works [9–11] about the relation of these two quantities.

2

In 2004 Hastings [9] showed that in any dimension, the ground state of a gapped Hamiltonian always presents exponential decay of correlations. Brandão and Horodecki showed [10] that for 1D systems, exponential decay of correlations implies *area law scaling* of the entanglement entropy. Thermal states also present exponential decay of correlations. These states, understood as a mixture of pure states present an apparent paradox concerning the behavior of their correlation functions. Due to typicallity arguments [12], random pure states are, with very high probability, maximally entangled, thus they do not fulfill *area laws* leading to a non-exponential decay of correlations; however, when we average over each instance in the thermal state we end up with a thermal density matrix and therefore an exponentially decaying signal in the correlation functions.

In this document we study spectral properties of reduced density matrices of the XY model and we explore the apparent paradox mentioned before for the quantum correlations based on previous works: (i) This model was introduced first by Lieb, Schultz and Mattis [13] to study the influence of symmetry in many-body systems. (ii) Barouch and McCoy [14, 15] presented a complete and extended work on the statistical mechanics of the XY model where they computed the asymptotic behavior of spin-spin correlation functions and showed that, for every temperature of the system, these correlations decay exponentially with the distance between the spins involved in the correlation function.

This document is divided into 5 chapters. In Chapter 2 we review three important results we need to properly state the problem we want to attack throughout this work: (i) The fact that every eigenstate of Hamiltonians quadratic in fermion operators is Gaussian so it can be characterized by its fermionic covariance matrix. (ii) The relation between the scaling behavior of entanglement entropy and correlation functions. (iii) Canonical typicallity. In Chapter 3 we present some standard results for the XY model and some properties of the fermionic

covariance matrix. This chapter ends with the calculation of fluctuation matrix of the fermionic covariance matrix. In Chapter 4 we present the numerical results for the spatial structure of the entanglement entropy for the ground state in critical and non-critical regimes. Also this spatial structure is studied for macroscopically excited states and we show the numerical calculations for the fluctuations in the reduced fermionic covariance matrix for thermal states. Chapter 5 contains the conclusions of the work.

2

Theoretical background

In this chapter we introduce the concepts of quasi-free fermionic models on a lattice and present Majorana fermions to define the fermionic covariance matrix. We also comment on the relation of entanglement entropy and correlation functions in 1-dimensional systems. We present the 'thermal canonical principle' which allows us to state the problem of the apparent paradox in the correlation functions for thermal states.

2.1 Fermionic quadratic Hamiltonians

In many-body physics, most of models are difficult if not impossible to solve. Also a large set of complicated Hamiltonians representing interacting systems can be mapped, under appropriate approximations (or transformations), to Hamiltonians quadratic in fermionic operators

of the form

$$H = \sum_{i,j}^{N} C_{ij} b_i b_j + \sum_{i,j}^{N} (A_{ij} b_i^\dagger b_j^\dagger + \text{h.c.}), \qquad (2.1)$$

where N is the number of modes and $b_i^\dagger$, b_i are fermionic creation and annihilation operators respectively, satisfying canonical anticommutation relations of the form

$$\{b_i^\dagger, b_j^\dagger\} = \{b_i, b_j\} = 0, \quad \{b_i^\dagger, b_j\} = \delta_{ij}, \qquad (2.2)$$

where, $\{A, B\} := AB + BA$, the anticommutator of A and B.

Important classes of models that are described in terms of Hamiltonians like (2.1) are Hubbard models [16], the BCS theory of superconductivity in the *mean field* approximation [17] and spin chains after a Jordan-Wigner transformation (which is the most relevant class for this work) [16, 18]. Hamiltonians of the generic form of (2.1) are diagonalized through Bogoliubov transformations (i.e., canonical transformations). These transformations map interacting fermions into noninteracting quasi-particles (fermions) that are expressible as a linear combination of the creation and annihilation operators b, $b^\dagger$; that is,

$$\tilde{b}_i = u_i^j b_j + v_i^j b_j^\dagger, \qquad (2.3)$$

where u_i^j and u_i^j are complex numbers restricted by the fact that (2.3) must preserve the canonical anticommutation relations stated in (2.2) for $\tilde{b}$ and $\tilde{b}^\dagger$.

Hamiltonians with the generic form of (2.1) have the interesting properties that not only the ground state but *every* eigenstate representing a certain number of excitations of quasi-particles, described by $\tilde{b}$ and $\tilde{b}^\dagger$, belong to the so-called class of *fermionic Gaussian states*, which is a very nice property since it allows us characterize them in terms of

second order correlations because all the higher moments factorize as stated in Wick's theorem [19]. An equivalent but convenient characterization of second order correlations are defined in terms of Majorana fermions as we will see bellow.

2.1.1 MAJORANA FERMIONS

Majorana fermions are represented by $2N$ hermitian operators defined as

$$\gamma_j = b_j^\dagger + b_j, \quad \gamma_{j+N} = (-i)(b_j^\dagger - b_j), \tag{2.4}$$

where for each fermion labeled by j of the original system we define the two operators above. The canonical anticommutation relations take the form

$$\{\gamma_\alpha, \gamma_\beta\} = 2\delta_{\alpha\beta}, \tag{2.5}$$

which is called a *Clifford algebra*[1]. After changing from fermions described by the operators $b^T := (b_1, b_2, \ldots, b_N, b_1^\dagger, b_2^\dagger, \ldots, b_N^\dagger)$ to Majorana operators $\gamma^T := (\gamma_1, \gamma_2, \ldots, \gamma_N, \gamma_{1+N}, \gamma_{2+N}, \ldots, \gamma_{2N})$, it is convenient to define the *fermionic covariance matrix* which completely specifies *fermionic Gaussian states*.

---

[1]The orthogonal group in $2N$ dimensions $O(2N)$ preserves the *Clifford algebra* hence the canonical anticommutation relations of fermionic operators [see [20] for fhurther details].

2.1.2 Fermionic Gaussian states and fermionic covariance matrix

Gaussian states are completely characterized by second moments [17] , that is the density matrix can be written as

$$\rho = \frac{1}{Z} \exp\left[-\frac{i}{4}\gamma^T G \gamma\right], \qquad (2.6)$$

where Z is a normalization constant, $\gamma^T = (\gamma_1, \ldots, \gamma_{2N})$ is the vector of Majorana fermions and G is a real antisymmetric $2N \times 2N$ matrix. Since G is antisymmetric, it is possible to put it in the form

$$OGO^T = \begin{bmatrix} 0 & -\tilde{B} \\ \tilde{B} & 0 \end{bmatrix}, \qquad (2.7)$$

where $\tilde{B}$ is diagonal, with eigenvalues that we denote by β_k) and $O \in O(2N)$. The right hand side of (2.7) is known as the Williamson form of the antisymmetric matrix G and $\tilde{\beta}_k$ are the Williamson eigenvalues of G.

It is convenient to characterize second order correlations in terms of the so-called *fermionic covariance matrix* (FCM), whose entries are

$$\Gamma_{\alpha\beta} = \frac{1}{2i} \operatorname{tr}(\rho[\gamma_\alpha, \gamma_\beta]), \qquad (2.8)$$

where $[\gamma_\alpha, \gamma_\beta] := \gamma_\alpha \gamma_\beta - \gamma_\beta \gamma_\alpha$ and $\alpha, \beta = 1, \ldots, 2N$. Again it is possible to find an orthogonal transformation $O \in O(2N)$ that brings Γ to its Williamson form $\tilde{\Gamma}$; that is

$$\tilde{\Gamma} = O\Gamma O^T = \begin{bmatrix} 0 & -\operatorname{diag}(\lambda_k) \\ \operatorname{diag}(\lambda_k) & 0 \end{bmatrix}, \qquad (2.9)$$

where the $\lambda_k = \tanh(\beta_k/2)$ for $k = 1, \ldots, N$ [21] which determines the connection between the matrix G in (2.6) and the *fermionic covariance*

8

matrix Γ. The Williamson eigenvalues are $\lambda_k = n_k - \frac{1}{2}$, where n_k is the fermion occupation number of the normal mode labeled by k.

The $O(2N)$ equivalence of fermion Gaussian states leads to the nice property stated above about the 'Gaussianity' of states describing quasiparticle excitations. Suppose $|\text{vac}\rangle$ is the ground state of (2.1), thus $b_i |\text{vac}\rangle = 0$, $\forall i = 1, \ldots, N$. This together with the definition (2.4) implies that $b_i^\dagger |\text{vac}\rangle = \gamma_i |\text{vac}\rangle$. Therefore the multiparticle states are obtained from some transformation of the ground state $|\text{vac}\rangle$ that preserves the anticommutation relations of the fermionic operators, and since this state is Gaussian, the resulting one will also be Gaussian.

The fact that all eigenstates of the Hamiltonian in (2.1) are Gaussian is very important since in this work we focus our attention in studying the structure of the FCM of excited states of the XY model.

2.2 ENTANGLEMENT AND CORRELATION FUNCTIONS

The number of degrees of freedom involved in describing a general state of a many-body quantum system grows exponentially with the number of constituents of the systems. This makes computing the explicit form of the eigenstates of fermionic quadratic Hamiltonians complicated enough to then study entanglement properties.

Even though ground states of some specific models have been previously computed, studying entanglement for these states may represent computational difficulties since they may depend on a exponential number of coefficients on a given basis. On the other hand, conceptually it is also a challenging task because entanglement of large number of particles has not been established what aspects of the states a sensible characterization should consider [16].

In the following we motivate our particular approach to the problem of studying correlations of the ground state and macroscopically

excited states (MES)[2] in terms of spectral properties of the reduced density matrix of sub-systems and in particular its entropy. As stated previously it is important that all eigenstates of the type of Hamiltonians studied here are *fermionic Gaussian states*, thus the entropy of these states is computed easily from the Williamson spectrum of its correspondent *fermionic covariance matrix*, which represents a significant reduction of the parameters needed to characterize the state. We start with a very brief review on previous works.

2.2.1 Bipartite entanglement

Bipartite entanglement have been extensively studied, in particular by Bennett et al. [22]. The theory of bipartite entropy is based on the possibility of converting one entangled state ρ into another state ρ' by applying LOCC (Local Operations and Classical Communication) transformations [23]. If the transformation from ρ to ρ is possible with LOCC transformations then ρ cannot be more entangled than ρ' since LOCC can only introduce classical correlations, thus the local convertibility of ρ into ρ' can be used to compare the amount of entanglement in different states.

Even though the general case of entanglement in systems with $S > 2$ subsystems is not well understood, in the particular case of $S = 2$ subsystems (A and its compliment B), and for pure states, there is enough work supporting the idea that bipartite pure-state entanglement can be characterized by the entanglement entropy $S(\rho)$ [16]. The entanglement entropy makes sense only after a bipartition of the full system and is the von Neumann entropy of the reduced density matrix $\rho_A := \mathrm{tr}_B \rho$, where tr_B means tracing out the degrees of freedom of the

---

[2]Eigenstates of the Hamiltonian (2.1) representing a number of excitation of quasi-particles

complementary system B of the subsystem A, that is,

$$S(\rho) = -\operatorname{tr}(\rho_A \log \rho_A). \qquad (2.10)$$

The results obtained in the literature for bipartite entanglement are sufficient for the purposes of this work.

2.2.2 ENTROPY OF A BLOCK OF SITES

We are interested in systems described by the Hamiltonian (2.1) representing N sites that can be occupied by interacting fermions. Particularly one can be interested in quantum correlations between a partition of the whole system into two subsystems that are blocks of adjacent sites of sizes L and $N - L$ respectively. This approach was proposed by Vidal et al. [24] to explore the behavior of quantum correlations at different length scales dictated by the size, L, of the block (sub-system) and capture some universal properties near critical points.

For a pure state, ρ, of the system we will say that S_L is the entanglement entropy between the block and its compliment, that is

$$S_L = -\operatorname{tr}(\rho_L \log \rho_L), \qquad (2.11)$$

where $\rho_L = \operatorname{tr}_{N-L} \rho$, with tr_{N-L} representing the trace over the $N - L$ sites remaining in the full system. It is important to notice that we are dealing with translationally invariant states since the ρ_L depends only in the number of sites involved and not in the position in the system. In fig.(2.2.1) we depict the situation stated above.

At first sight one may think that the entropy of entanglement S_L must have an extensive character, that is, since it is encoding information about the quantum correlations between the sites in the block and the sites in its compliment it must grow with the number of sites L that

L sites

$$\rho_L \rightarrow S_L$$
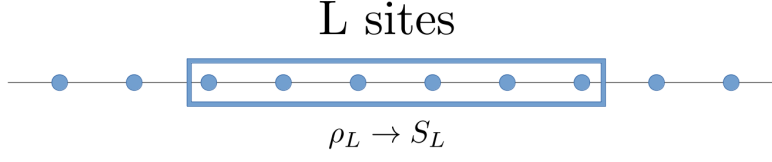
Figure 2.2.1: The entropy of entanglement S_L is the von Neumann entropy of the reduced density matrix ρ_L of the block of sites depicted here. It measures the amount of entanglement between this block and the rest of the sites for a pure state.

make up the chain. This extensive behavior is referred as *volume law scaling* of entanglement entropy observed in thermal states [11, 25–27]. Remarkably, for ground states, typically one finds that S_L grows with the boundary of the block rather than its volume, then it is said that the entanglement entropy fulfills an *area law*[9] because it is merely linear with the size of the boundary of the block of L sites.
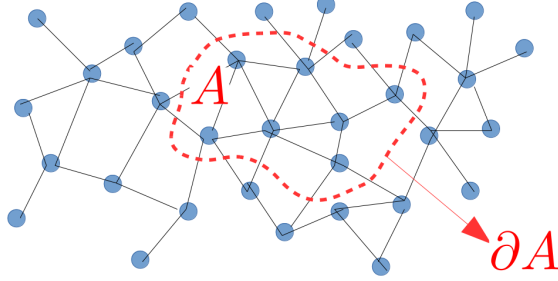
Figure 2.2.2: Each point on the lattice represents a particle, the links represent the interaction between sites and the red dashed line encloses the A region. *Volume law* scaling states that the entropy grows with the number of points inside A. *Area law* scaling states that the entropy grows with the boundary ∂A, that is, it grows with the number of links crossed by the dashed line.

2.2.3 Correlation functions

The scaling behavior of entanglement entropy has important and non-trivial consequences in the distribution of quantum correlations in quantum many-body systems. Intuitively if the entropy of entanglement follows a *volume law* we may think that every mode in the block is entangled with the rest of the modes in the complementary block, hence the proportionality with L as we will show later in this work. On the contrary, *area law scaling* comes with the additional property of exponential decay of correlation functions (also known as the exponential clustering property) for local Hamiltonians [see [11]]. The implication of *area law* from exponential decay of correlations is not obvious and also is not proven for arbitrary dimensions. In 2015 Brandão and Horodecki showed that for 1-dimensional quantum states the exponential decay of correlations[3] implies area-law in their entanglement entropy [10].

The theorem presented by Brandão and Horodecki is one of the main results used to state the problem we are interested in this work since we work with the 1-dimensional XY model.

In order to properly state the problem we want to address in this document we need a another main result regarding on typicality of quantum states.

2.3 Canonical typicallity

The following results are discused in detail in the work of Popescu, Short and Winter [12]. Again we consider a bipartition into S for our *system* of interest and E its compliment (the *environment*) of a big system referred as the *universe* and. In the general case we are interested in a Hilbert space that is a subspace of the tenser product

---

[3]The correlations used in the original (1.1) work generalize the idea of two-point correlators that are essentially the entries of the FCM presented in the previous section.

of the form $\mathcal{H}_R = \mathcal{H}_S \otimes \mathcal{H}_E$; here $\mathcal{H}_S$ and $\mathcal{H}_E$ are the Hilbert spaces of the system and the environment respectively and R represents a certain physical restriction (e.g. the total energy of the *universe* is constant). The state of the *universe* representing the mixture of equal probability pure states is

$$\mathcal{E}_R = \frac{\mathbb{1}_R}{d_R}, \tag{2.12}$$

being $\mathbb{1}_R$ the identity on $\mathcal{H}_R$ and $dim(\mathcal{H}_R) = d_R$.

The canonical state of the *system*, Ω_S, for the restriction R, is obtained by tracing out the degrees of freedom of the *environment* in the equiprobable state of the *universe*, that is

$$\Omega_s = \mathrm{tr}_E \, \mathcal{E}_R. \tag{2.13}$$

The important result showed by Popescu et al. states that if the *universe* is in a pure state, $|\Phi\rangle$, and $\rho_S = \mathrm{tr}_E |\Phi\rangle \langle\Phi|$ is the correspondent state of the *system*, then we have that the for almost every pure state $|\Phi\rangle \in \mathcal{H}_R$ of the *universe*, the *system* is in the canonical state (2.13) consistent with the restriction R. The previous result is stated as.

$$\rho_S \approx \Omega_S. \tag{2.14}$$

This is known in the literature as the canonical principle. It is important to notice that the previous results are hold for general restrictions, R. Also, as long as the *system* is 'small' compared with the *universe*, as we will use after in this document the *universe* here may represent an isolated system of spins or fermions in a lattice, the *system* then could be a block of adjacent sites and the *environment* would be its complimentary block.

Now we set the restriction R, to the usual constraint used in standard statistical mechanics; namely that the total energy of the *universe* is

14

close to a given number ε. Considering that the total Hamiltonian of the universe H_U is

$$H_U = H_S + H_E + H_{\mathrm{int}} \qquad (2.15)$$

where H_S is the Hamiltonian of the *system*, H_E is the Hamiltonian of the *environment* and H_{int} is the interaction Hamiltonian. For the purpose of this document, the interaction Hamiltonian depends on operators acting on the boundary modes of the sub-region whereas H_S and H_E depend on many more operators, then H_{int} is small compared with the other two Hamiltonians in (2.15). Thus almost every pure state of the *universe* is such that the *system* is in the thermal canonical state

$$\Omega_S^{(\varepsilon)} \propto \exp[-\beta H_S], \qquad (2.16)$$

where β is the inverse temperature scale set by the restriction R, for the energy of the *universe*. The previous result is known as the thermal canonical principle. For details on this result see [12].

We will use this typicality argument in the following section to properly state the problem we want to address in this document.

2.4 STATEMENT OF THE PROBLEM

We will now turn to the main object of study of this document; the two-point correlation functions of eigenstates of the 1-dimensional XY model encoded in the entries of the fermionic covariance matrix. Remember that the characterization of the quantum correlations of these states is possible in term of their FCM because the belong to the general class of fermionic Gaussian states.

Due to canonical typicality arguments, the random pure states drawn from the uniform spherical measure, give rise to sub-systems that are

very nearly maximally entangled with their complementary sub-system. This is manifested in the *volume law* fulfilled by entanglement entropy. We shall show this extensive property of the entropy of entanglement in macroscopically excited states of the XY model.

In 1-dimensional quantum systems, the implication of *area law* for entanglement entropy in states that fulfill exponential decay of correlations presented by Brandão and Horodecki [10] is that if a state has entanglement entropy that fulfills a *volume law*, then it must have no exponential decay of correlations.

Canonical typicality assures that the full system is in a thermal state ρ that can be understood as a mixture of pure states $|\Phi_\alpha\rangle$, that is

$$\rho = \sum_\alpha p_\alpha |\Phi_\alpha\rangle \langle\Phi_\alpha| . \qquad (2.17)$$

We will ague that thermal states such as ρ have exponential decay of correlations but each of its constituents does not have this exponential clustering property because do not fulfill *area law scaling* of entanglement entropy.

It is remarkable that each of the constituents of ρ do not present exponential decay of correlations but somehow when the mixture is done the non-exponential behavior of each contribution to the correlations must cancel resulting in an exponentially decaying signal. In summary, at sufficiently large distances, the fluctuations generated by each instance of the thermal state in the correlation functions must cancel with other contributions so that the result is an exponential decay of correlations for the state ρ.

2.4.1 STRUCTURE OF THE METHODOLOGY

As we will show in the following chapter, we start with the 1D XY model and transform it to a Hamiltonian of the form of (2.1). We devote our

study to the spectral properties of the fermionic covariance matrices that, as we argued before, is sufficient to characterize eigenstates of this Hamiltonian.

The FCM of a thermal state is generated as a superposition of states representing a given number of quasi-particle excitations. Since we want to study the apparent paradox in the behavior of correlation functions of a thermal state in relation with its individual constituents, we study the fluctuations around the mean covariance matrix that must provide the information about the previously mentioned cancellation for long distances and then resulting in an exponentially decaying signal in the correlation functions.

In this chapter we have argued that all eigenstates of fermionic quadratic Hamiltonians belong to the general class of fermionic Gaussian states and therefore they are completely characterized by its fermionioc covariance matrix. Also we have mentioned the connection between the scaling nature of entanglement entropy and the behavior of correlation functions. Finally we have presented a typicallity argument which assures that a random pure state is, with very high probability, a maximally entangled state. In the next chapter we present the XY model and compute discuss some properties of the fermionic covariance matrix.

3

The XY model

In this chapter we present some preliminaries on the 1D XY model. We develop some standard calculations on the diagonalization of the Hamiltonian after a series of transformations based on previous works. The first exact solution for the XY model, for magnetic field $\lambda = 0$, was presented by Lieb, Schultz and Mattis [13]. Then Katsura [28] computed the spectrum of the XY model for $\lambda \neq 0$ and Barouch and McCoy presented 4 papers on the statistical mechanics of the XY model where they compute, among other things, the two-point correlation functions for arbitrary values of the parameters γ and λ in states at inverse temperature β. Results on the structure of entanglement entropy, S_L, for a block of L adjacent spins was first computed by Vidal et al. [24]. Here we mention some basic aspects on the criticallity of this model [see [16] for further details]. This chapter finishes with a discussion

on the fluctuations around the mean fermionic covariance matrix for macroscopically excited states in the full chain and in a block of spins.

3.1 THE XY HAMILTONIAN

The XY Hamiltonian models a set of N spin-1/2 particles located on the sites of a $d-$dimensional lattice. In the rest of this document we will refer to the 1D XY model simply as the XY model.

We have a chain of N spins where each spin is able to interact with its nearest neighbors and with an external magnetic field, mathematically the Hamiltonian representing this situation reads

$$H_{XY}^{(N)} = -\frac{1}{2} \sum_{l=0}^{N-1} \left(\frac{1+\gamma}{2} \sigma_l^x \sigma_{l+1}^x + \frac{1-\gamma}{2} \sigma_l^y \sigma_{l+1}^y + \lambda \sigma_l^z \right), \qquad (3.1)$$

where γ is the so-called anisotropy parameter and represents the difference between the strength of the $xx-$interaction and the $yy-$interaction (in spin space) and λ is the intensity of the external magnetic field. On the other hand

$$\sigma_l^i = \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes \underbrace{\sigma^i}_{\text{site } l} \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}, \qquad (3.2)$$

and σ^i are Pauli matrices for $i = x, y, z$,

$$\sigma^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma^y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \qquad (3.3)$$

The XY model has been widely studied since for some specific values of the parameters γ and λ or some limits it correspond to other models of interest in condensed matter physics. Some examples are the following: (i) the boson Hubbard model in the in the limit of hard bosons [16]. (ii) For $\gamma = 1$ (3.1) corresponds to the Ising model. (iii) The Kitaev

19

chain is equivalent to the XY model under an proper identification of the parameters μ, t and Δ with γ and λ [29].

3.1.1 THE SPECTRUM

To find the spectrum of the Hamiltonian (3.1) of the XY model it is necessary to perform three different transformations. These results are very standard and we present them here to make the discussion self consistent.

JORDAN-WIGNER TRANSFORMATION

We first consider the non-local transformation given by

$$b_l = \left(\prod_{m<l} \sigma_m^z\right) \sigma_l^-, \quad \sigma_l^- = \frac{\sigma_l^x - i\sigma_l^y}{2}; \tag{3.4}$$

these b_l represent spinless fermionic operators because they follow canonical anticommutation relations

$$\{b_l^\dagger, b_k^\dagger\} = \{b_l, b_k\} = 0, \quad \{b_l^\dagger, b_k\} = \delta_{lk}. \tag{3.5}$$

After this transformation, the Hamiltonian becomes

$$H_{XY}^{(N)} = \frac{1}{1}\sum_{l=0}^{N-1}[(b_{l+1}^\dagger b_l + \text{h.c.}) + \gamma(b_l^\dagger b_{l+1}^\dagger + \text{h.c.})] - \lambda\sum_{l=0}^{N-1} b_l^\dagger b_l, \tag{3.6}$$

which is a Hamiltonian that has the generic form (2.1) mentioned at the beginning of the previous chapter.

FOURIER TRANSFORMATION

If we consider periodic boundary conditions (PBC), that is, we identify the spin in site N with the spin in site 1 then we can Fourier transform

the operators b_l in the following way

$$d_k = \frac{1}{\sqrt{N}} \sum_{l=0}^{N-1} e^{-i\theta_k l} b_l, \quad \theta_k = \frac{2\pi}{N} k. \tag{3.7}$$

Since this Fourier transformation is unitary, the operators d_k are fermionic operators with anticommutation relations.

In terms of d_k operators the Hamiltonian takes the form

$$H_{XY}^{(N)} = \sum_{k=-(N-1)/2}^{(N-1)/2} (-\lambda + \cos\theta_k) \, d_k^\dagger d_k + \frac{i\gamma}{2} \sum_{k=-(N-1)/2}^{(N-1)/2} \sin\theta_k (d_k d_{-k} + \text{h.c.}),$$

$$\tag{3.8}$$

where we have suppressed an additional term that is proportional to $1/N$ since we will be interested in the limit $N \to \infty$.

Bogoliubov (canonical) transformation

Now we consider a canonical transformation as mentioned in (2.3) for the d_k operators

$$\tilde{d}_k = u_k d_k^\dagger + i v_k d_{-k}. \tag{3.9}$$

Since we want this transformation to preserve the canonical anticommutation relations we need that $u_k^2 + v_k^2 = 1$ then we can use the parametrization $u_k = \cos(\psi_k/2)$ and $v_k = \sin(\psi_k/2)$ given by

$$\cos(\psi_k) = \frac{-\lambda + \cos\theta_k}{\sqrt{(\lambda - \cos\theta_k)^2 + (\gamma \sin\theta_k)^2}}, \tag{3.10}$$

21

and with this transformation the Hamiltonian takes the diagonal form

$$H_{XY}^{(N)} = \sum_{k=-(N-1)/2}^{(N-1)/2} \tilde{\Lambda}_k \tilde{d}_k^\dagger \tilde{d}_k \qquad (3.11)$$

with

$$\tilde{\Lambda}_k := \sqrt{(\lambda - \cos\theta_k)^2 + (\gamma\sin\theta_k)^2}. \qquad (3.12)$$

Finally, defining $\theta := 2\pi k/N$ and taking the thermodynamic limit $N \to \infty$, the spectrum of the XY model is

$$\Lambda(\theta) := \sqrt{(\lambda - \cos\theta)^2 + (\gamma\sin\theta)^2}. \qquad (3.13)$$

3.1.2 THE XY MODEL IN PARAMETER SPACE

We can use the expression (3.13) for the spectrum to identify regions in the (γ, λ)−plane where the XY model presents critical behavior.

The quantity that encodes the criticallity of the model is the correlation length ξ that characterizes the exponential decay of spin-spin correlations

$$\left\langle [\sigma_l^i, \sigma_{l+R}^i] \right\rangle \sim e^{-\frac{R}{\xi}}. \qquad (3.14)$$

Near critical points, this correlation length diverges. Distinct behaviors are present for this divergence, one for $\gamma = 0$ and $\lambda = (0, 1]$ and another for $\lambda = 1$ [15, 16]. Barouch and McCoy showed that in the line $\gamma^2 + \lambda^2 = 1$ there is also a divergence in the correlation length. In fig.(3.1.1) we show the critical regions in the XY model in the parameter space.

We will see in the next chapter that these results are important when we show the scaling nature of the entanglement entropy with the size
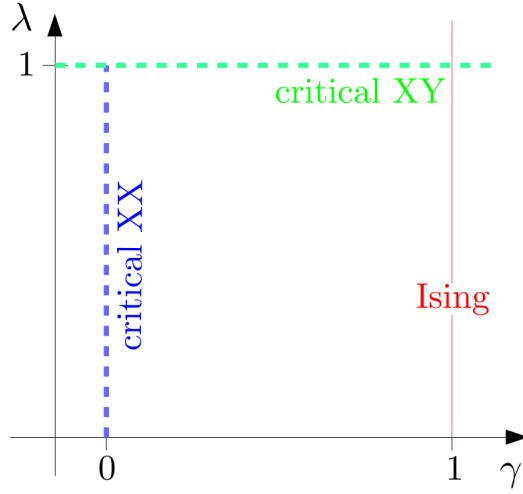
Figure 3.1.1: Parameter space of the XY model. The blue line, $\gamma = 0$, corresponds to the XX model which is critical for $\lambda \in (0, 1]$. The line, $\lambda = 1$, correspond to the critical XY model.

of the block.

3.2   FCM of the XY model

Since we devote our analysis on the structure of entanglement entropy and quantum correlations to the study of spectral properties of reduced density matrices of eigenstates of Hamiltonians quadratic in fermion operators (that are Gaussian), it is important to characterize the fermionic covariance matrix of the XY model. In order to do that we need to express the Hamiltonian (3.1) in terms of Majorana fermions using an analogous Jordan-Wigner transformation to the one used to diagonalize the XY Hamiltonian but into $2N$ Majorana fermions

$$\gamma_l = \left(\prod_{m<l} \sigma_m^z \right) \sigma_l^x, \quad \gamma_{l+N} = \left(\prod_{m<l} \sigma_m^z \right) \sigma_l^y, \qquad (3.15)$$

where again $l = 10, \ldots, N-1$.

Note the three following products:

$$
\gamma_l \gamma_{l+N} = \underbrace{\left(\prod_{m<l} \sigma_m^z\right) \left(\prod_{m<l} \sigma_m^z\right)}_{\mathbb{1}^{\otimes(l-1)}} \sigma_l^x \sigma_l^y = i\sigma_l^z, \tag{3.16}
$$

$$
\gamma_{l+N} \gamma_{l+1} = \left(\prod_{m<l} \sigma_m^z\right) \sigma_l^y \left(\prod_{m<l+1} \sigma_m^z\right) \sigma_{l+1}^x = \sigma_l^y \sigma_l^z \sigma_{l+1}^x = i\sigma_l^x \sigma_{l+1}^x \tag{3.17}
$$

and

$$
\gamma_l \gamma_{l+1+N} = \left(\prod_{m<l} \sigma_m^z\right) \sigma_l^x \left(\prod_{m<l+1} \sigma_m^z\right) \sigma_{l+1}^y = \sigma_l^x \sigma_l^z \sigma_{l+1}^y = -i\sigma_l^y \sigma_{l+1}^y, \tag{3.18}
$$

which are, up to constant factors, the three term ins (3.1); then we can write XY Hamiltonian as

$$
H_{XY}^{(N)} = \frac{i}{4} \sum_{\alpha,\beta=0}^{2N} \Omega_{\alpha\beta} [\gamma_\alpha, \gamma_\beta], \tag{3.19}
$$

where Ω is the antisymmetric matrix of the form

$$
\Omega = \begin{bmatrix} 0 & \Omega^{(0)} \\ -\Omega^{(0)} & 0 \end{bmatrix} \tag{3.20}
$$

24

where

$$\Omega^{(0)} = \begin{bmatrix} 2\lambda & -(1-\gamma) & & & 1+\gamma \\ 1+\gamma & 2\lambda & -(1-\gamma) & & \\ & \ddots & \ddots & \ddots & \\ & & 1+\gamma & 2\lambda & -(1-\gamma) \\ -(1-\gamma) & & & 1+\gamma & 2\lambda \end{bmatrix}. \quad (3.21)$$

Given that $\Omega^{(0)}$ is a circulant and real matrix, it can be diagonilized by means of a Fourier transformation. Therefore it can be written as

$$\Omega^{(0)}_{nm} = \frac{1}{N} \sum_{\theta_k} \omega(\theta_k) e^{i\phi(\theta_k)} e^{i(m-n)\theta_k} = \frac{2}{N} \sum_{\theta_k=0}^{\pi} \omega(\theta_k) \cos\left((n-m)\theta_k + \phi(\theta_k)\right).$$

$$(3.22)$$

where

$$\omega^2(\theta_k) := (\lambda - \cos\theta_k)^2 + \gamma^2 \sin^2\theta_k \quad (3.23)$$

and

$$\phi(\theta_k) := \arctan\left(\frac{\lambda - \cos\theta_k}{-\gamma \sin\theta_k}\right). \quad (3.24)$$

The first summation in (3.22) is understood over k with $-(N-1)/2 \leq k \leq (N-1)/2$ which is equivalent to $-\pi \leq \theta_k \leq \pi$. Let us define the following functions

$$u_m^c(\theta_k) = \sqrt{\frac{2}{N}} \cos(m\theta_k + \phi(\theta_k)), \quad (3.25)$$

$$u_m^s(\theta_k) = \sqrt{\frac{2}{N}} \sin(m\theta_k + \phi(\theta_k)), \quad (3.26)$$

25

$$v_m^c(\theta_k) = \sqrt{\frac{2}{N}} \sin(m\theta_k), \tag{3.27}$$

$$v_m^s(\theta_k) = \sqrt{\frac{2}{N}} \sin(m\theta_k) \tag{3.28}$$

to rewrite $\Omega_{nm}^{(0)}$ as

$$\Omega_{nm}^{(0)} = \sum_{\theta_k=0}^{\pi} \omega(\theta_k)[u_m^c(\theta_k)v_n^c(\theta_k) + u_m^s(\theta_k)v_n^s(\theta_k)] \tag{3.29}$$

so the upper right block of (3.19), $H^{(N)}$, is

$$H^{(N)} = \sum_{n,m=0}^{N-1} \frac{i}{4} \sum_{\theta_k=0}^{\pi} \omega(\theta_k)[u_m^c(\theta_k)v_n^c(\theta_k) + u_m^s(\theta_k)v_n^s(\theta_k)][\gamma_n, \gamma_{m+N}],$$

$$\tag{3.30}$$

and rearranging things we get

$$H^{(N)} = \frac{i}{4} \sum_{\theta_k=0}^{\pi} \omega(\theta_k)(\underbrace{[\gamma_k^c, \gamma_{k+N}^c]}_{1-2\sigma_k^z} + \underbrace{[\gamma_k^s, \gamma_{k+N}^s]}_{1-2\sigma_k^z}), \tag{3.31}$$

where

$$\gamma_k^{c,s} := \sum_n u_n^{c,s}(\theta_k)\gamma_n, \quad \gamma_{k+N}^{c,s} := \sum_n v_n^{c,s}(\theta_k)\gamma_{n+N}. \tag{3.32}$$

Now we recall that the fermionic covariance matrix is defined as in (2.8), then the transformation that brings the Ω into its Williamson does the same on the FCM. Thus the upper-right block of FCM, in

position space, is

$$M_{mn} = \sum_{\theta_k=0}^{\pi} [m^c(\theta_k)u_m^c(\theta_k)v_n^c(\theta_k) + m^s(\theta_k)u_m^c(\theta_k)v_n^c(\theta_k) + m^s(\theta_k)]$$

(3.33)

where $m^{c,s}(\theta_k) = n^{c,s}(\theta_k) - \frac{1}{2}$, being $n^{c,s}(\theta_k)$ the 'cosine' ('sine') fermion occupation number of the mode labeled by k. It is convenient to rewrite the FCM as

$$M_{mn} = \sum_{\theta_k=0}^{\pi} \left(\frac{m^c(\theta_k) + m^s(\theta_k)}{2} \right) (u_m^c(\theta_k)v_n^c(\theta_k) + u_m^s(\theta_k)v_n^c(\theta_k))$$
$$+ \sum_{\theta_k=0}^{\pi} \left(\frac{m^c(\theta_k) - m^s(\theta_k)}{2} \right) (u_m^c(\theta_k)v_n^c(\theta_k) - u_m^s(\theta_k)v_n^c(\theta_k)).$$

(3.34)

Now let $m^{\pm}(\theta_k) = (m^c(\theta_k) \pm m^s(\theta_k))/2$. We can undo the transformation from (3.22) to (3.29) to have

$$M_{mn} = \underbrace{\sum_{\theta_k=-\pi}^{\pi} m^+(\theta_k)e^{i\phi(\theta_k)}e^{i(n-m)\theta_k}}_{:=M_{mn}^+} + \underbrace{\sum_{\theta_k=-\pi}^{\pi} m^-(\theta_k)e^{i\phi(\theta_k)}e^{i(n+m)\theta_k}}_{:=M_{mn}^-} .$$

(3.35)

For the matrix M^- one can relable the index $n \to -n'$. In this way both the circulant and the anticirculant[1] parts of M are computed as

---

[1] We say a matrix A is anticirculant if it has the form

$$A = \begin{pmatrix} a_1 & a_2 & \cdots & a_{N-1} & a_N \\ a_2 & a_3 & \cdots & a_N & a_1 \\ \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \cdot^{\cdot^{\cdot}} & \cdots & \cdot^{\cdot^{\cdot}} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ a_N & a_1 & a_2 & \cdots & a_{N-1} \end{pmatrix}$$

(3.36)

Fourier transformations of the vectors $m^+(\theta_k)e^{i\phi(\theta_k)}$ and $m^-(\theta_k)e^{i\phi(\theta_k)}$ respectively.

Here we note two things: (i) The FCM always can be written as a circulant matrix M^+ plus an anticirculant matrix M^-. (ii) For the ground state, the FCM is circulant because the fermion occupation numbers $n^c(\theta_k) = n^s(\theta_k) = 0$, $\forall k$.

3.2.1 Fluctuations in the FCM for macroscopically excited states

As we mentioned before, it is important to study the thermodynamic fluctuations around the mean FCM because they are responsible for the exponential decay of quantum correlations in thermal states of the XY model. We consider an ensemble of fermionic covariance matrices at inverse temperature β generated using the fermion occupation numbers $n^c(\theta_k)$, $n^s(\theta_k)$ and a Fermi-Dirac distribution

$$\nu(\theta_k) := \Pr(n^{c,s}(\theta_k) = 1) = \frac{1}{e^{\beta\omega(\theta_k)} + 1}, \tag{3.37}$$

where $\Pr(n^{c,s}(\theta_k) = 1)$ is the probability of the occupation number $n^{c,s}(\theta_k)$ to be 1. Let us denote by $\Delta M^\pm$ the matrix representing the difference from the mean sample matrix $\bar{M}^\pm$. Thus the fluctuations in this matrix are due to the fluctuations in the numbers $n^{c,s}(\theta_k)$, that is

$$(\Delta M^\pm)_{mn} = 2 \sum_{\theta_k=0}^{\pi} \left(\frac{\Delta n^c(\theta_k) \pm \Delta n^s(\theta_k)}{2} \right) \cos\left((m \mp n)\theta_k + \phi(\theta_k)\right). \tag{3.38}$$

Then the fluctuation matrix has three terms

$$\left\langle (\Delta M^{\pm})_{mn}(\Delta M^{\pm})_{m'n'} \right\rangle = \frac{1}{2} \sum_{\theta_k=0}^{\pi} \left(\left\langle \Delta n^c(\theta_k)^2 \right\rangle + \left\langle \Delta n^s(\theta_k)^2 \right\rangle \right) \times$$

$$\times \cos\left((m \mp n)\theta_k + \phi(\theta_k)\right) \cos\left((m' \mp n')\theta_k + \phi(\theta_k)\right), \quad (3.39)$$

and

$$\left\langle (\Delta M^{+})_{mn}(\Delta M^{-})_{m'n'} \right\rangle = \frac{1}{2} \sum_{\theta_k=0}^{\pi} \left(\left\langle \Delta n^c(\theta_k)^2 \right\rangle - \left\langle \Delta n^s(\theta_k)^2 \right\rangle \right) \times$$

$$\times \cos\left((m + n)\theta_k + \phi(\theta_k)\right) \cos\left((m' - n')\theta_k + \phi(\theta_k)\right), \quad (3.40)$$

and using the Einstein's formula for the fluctuations in the average number occupation $\nu(\theta_k)$ we see that the crossing term vanishes since $\left\langle \Delta n^c(\theta_k)^2 \right\rangle = \left\langle \Delta n^s(\theta_k)^2 \right\rangle = \nu(\theta_k)(1 - \nu(\theta_k))$. The other terms have always combinations $m \mp n$; for the circulant matrix we define the band indices $b = m - n$ and $b' = m' - n'$ and analogously for the anticirculant matrix we define the antiband indices $a = m + n$ and $a' = m' + n'$.

Let us define the two contribution to the fluctuations of the ensemble of FCM $B_{bb'} := \left\langle (\Delta M^{+})_b \Delta M^{+})_{b'} \right\rangle$ and $A_{aa'} := \left\langle (\Delta M^{-})_a \Delta M^{-})_{a'} \right\rangle$. For the circulant matrix we have

$$B_{bb'} := \sum_{\theta_k=0}^{\pi} \left(\frac{\nu(\theta_k)(1 - \nu(\theta_k))}{2} \right) \cos\left(b\theta_k + \phi(\theta_k)\right) \cos\left(b'\theta_k + \phi(\theta_k)\right),$$

$$(3.41)$$

and for the anticirculant matrix

$$A_{aa'} := \sum_{\theta_k=0}^{\pi} \left(\frac{\nu(\theta_k)(1 - \nu(\theta_k))}{2} \right) \cos\left(a\theta_k + \phi(\theta_k)\right) \cos\left(a'\theta_k + \phi(\theta_k)\right).$$

$$(3.42)$$

At first sight we may think that they are the same matrix, but we

29

will see that when dealing with the FMC of sub-systems the indices b, b' and a, a' run over different values giving significant changes.

3.2.2 Fluctuations in the FCM for sub-systems

In position space, the $L \times L$ sub-matrix of M corresponds to the upper-right block of the FCM for the sub-system of those L adjacent fermions. From now on, in this section we will denote by a sub-index q a quantity that is function of the angle $\theta_q := 2\pi q/(2L - 1)$.

We focus our attention in the banded matrix $B^{(L)}$ that corresponds to a $L \times L$ block matrix of B. Here the indices of the matrix $B^{(L)}$ run from $-(L - 1)$ and $L - 1$. Now we consider the set of $(2L - 1)$ orthogonal vectors whose b components are

$$
\begin{aligned}
c_b(\theta_q) &= \cos{(b\theta_q + \phi_q)}, \quad \text{for } q = 0, 1, \ldots, L - 1, \\
s_b(\theta_q) &= \sin{(b\theta_q + \phi_q)}, \quad \text{for } q = 1, 2, \ldots, L - 1.
\end{aligned}
\tag{3.43}
$$

We are interested in the action of the matrix $B^{(L)}$ on these vectors. For the sake of simplicity we define

$$
p(\theta_k) = \left(\frac{\nu(\theta_k)(1 - \nu(\theta_k))}{2} \right) \cos{(b\theta_k + \phi(\theta_k))},
\tag{3.44}
$$

so that

$$
\sum_{b'} B_{bb'}^{(L)} c_{b'}(\theta_q) = \int_0^\pi \frac{d\theta}{2\pi} p(\theta) \sum_{b'} \cos(b'\theta + \phi) \cos(b'\theta_q + \phi_q),
\tag{3.45}
$$

where we have changed the summation over k for an integral because we are interested in the thermodynamic limit, where $\theta = 2\pi k/N$ for

$N \to \infty$. Rearranging some terms, (3.45) is written as

$$= \frac{1}{2} \int_0^\pi \frac{d\theta}{2\pi} p(\theta) \left(\cos(\phi + \phi_q) \underbrace{\sum_{b'} e^{ib'(\theta + \theta_q)}}_{=D_{L-1}(\theta + \theta_q)} + \cos(\phi - \phi_q) \underbrace{\sum_{b'} e^{ib'(\theta - \theta_q)}}_{=D_{L-1}(\theta - \theta_q)} \right),$$

$$(3.46)$$

where

$$D_n(x) := \frac{\sin\left(\left(n + \frac{1}{2}\right)x\right)}{\sin\left(\frac{x}{2}\right)} \tag{3.47}$$

is the Dirichlet kernel of order n. The integrand in the preveious expression is an even function of θ; then,

$$= \frac{1}{2} \int_{-\pi}^\pi \frac{d\theta}{2\pi} p(\theta) \left(\cos(\phi + \phi_q) D_{L-1}(\theta + \theta_q) + \cos(\phi - \phi_q) D_{L-1}(\theta - \theta_q) \right).$$

$$(3.48)$$

The convolution of a function f with the Dirichlet kernel of order n is the $n-$th degree Fourier series approximation of the function f, therefore (3.48) is

$$= \frac{1}{4} \left(e^{i\phi_q} \overbrace{\sum_{l=-(L-1)}^{L-1} g_l e^{-il\phi_q}}^{\approx g(-\theta_q)} + e^{-i\phi_q} \overbrace{\sum_{l=-(L-1)}^{L-1} h_l e^{-il\phi_q}}^{\approx h(-\theta_q)} \right.$$

$$\left. + e^{-i\phi_q} \underbrace{\sum_{l=-(L-1)}^{L-1} g_l e^{il\phi_q}}_{\approx g(\theta_q)} + e^{i\phi_q} \underbrace{\sum_{l=-(L-1)}^{L-1} h_l e^{il\phi_q}}_{\approx h(\theta_q)} \right) \approx p(\theta_q), \qquad (3.49)$$

where g_l and h_l are the Fourier coefficients of the functions $g(\theta) := p(\theta)e^{i\phi}$ and $h(\theta) := p(\theta)e^{-i\phi}$ respectively. The four sums in (3.49) are $(L-1)-$th order Fourier expansions of the the functions $g(\theta_q)$ and

31

$h(\theta_q)$.

In conclusion we have

$$\sum_{b'} B_{bb'}^{(L)} c_{b'}(\theta_q) \approx \left(\frac{\nu(\theta_q)(1 - \nu(\theta_q))}{2} \right) c_b(\theta_q), \qquad (3.50)$$

which tell us that the vectors $\boldsymbol{c}(\theta_q)$ are approximately eigenvectors of the matrix $B^{(L)}$ with eigenvalue $\nu(\theta_q)(1 - \nu(\theta_q))/2$. This approximation relies on how well the functions $g(\theta)$ and $h(\theta)$ are approximated by their respective $(L-1)-$th order Fourier series. The functions involved in the integral are well behaved functions of θ, thus according to Parseval's theorem they have exponentially decaying Fourier coefficients, so as long as $L - 1$ is 'big' compared with the correlation length ξ this approximation makes sense.

On the other hand, for the $\boldsymbol{s}(\theta_k)$ vectors a similar treatment can be done but in (3.46) we will get sines instead of cosines, leading to an odd function of θ in the integrand which makes impossible to write as an integral over the full circle and consequently find approximations in terms of $(L - 1)-$th order Fourier series. Nevertheless in the next chapter we will show numerically that all the $L - 1$ vectors $\boldsymbol{s}(\theta_k)$ are mapped to a single vector $\boldsymbol{r}$ telling us that the $B^{(L)}$ is a matrix of rank $L + 1$ thus showing some invariant properties of the FCM of the sub-system.

In this chapter we have presented the standard calculations on the spectrum of the XY model and its FCM. We have discussed some general aspects of the critical regions in the $(\gamma, \lambda)-$plane and we have shown that the fluctuations in the FCM can be understood as a banded matrix M^+ plus an antibanded matrix M^-. In the next chapter we present the scaling nature and spatial structure of entanglement entropy for the ground state of the XY model in critical and non-critical regions. Also we discuss the spatial structure of entropy of entanglement for macroscopically excited states and present the principal

component analysis performed to the set of FCMs of macroscopically excited states that constitutes thermal state to study the fluctuations around the mean FCM.

4

Results and Discussion

In this chapter we present the methodology we use to study the spatial structure of entanglement entropy for the ground state in different regimes as well as for macroscopically excited states of the 1D XY model.

Since every eigenstate of the Hamiltonian (3.1) belongs to the class of fermionic Gaussian state, we can characterize it completely with its fermionic covariance matrix. We showed in the previous chapter that the Williamson values of the FCM are related with the fermionic occupation number operators of the modes that diagonalize the upper-right block of the matrix Γ. We also present the principal component analysis (PCA) performed to the set of macroscopically excited states that constitute a thermal state of the XY model.

4.1 The ground state

In this section we are interested in the spatial mode structure of the entropy of entanglement for the ground state of the XY model. Computing S_L for a block of L adjacent spins requires the Williamson values of the reduced fermionic covariance matrix M_L of the sub-system. In order to generate a FCM for the ground state we follow the next steps:

- Given a set of parameters γ and λ we compute the orthogonal transformation that takes the Hamiltonian to its Williamson form.

- Generate the FCM with the relation between the Williamson values of the FCM and the occupation numbers, in this case all the occupation numbers are zero.

- Apply the inverse transformation found in the first step to write the FCM in the position space for the fermion operators.

- Take a $L \times L$ sub-matrix of the FCM. This matrix is the FCM, M_L, for the block in position space. The ground state is tanslational invariant so in particular we can take the first L rows and columns of the FCM for the full system.

- Find the two matrices $O^{(1)}$ and $O^{(2)}$ from the singular value decomposition that diagonalize M_L. The entanglement entropy can be expressed in terms of the singular values d_k of the matrix M_L[1].

- Compute the participation function $\varrho_{ij} = \frac{1}{2}\left(\left(O_{ij}^{(1)}\right)^2 + \left(O_{ij}^{(2)}\right)^2\right)$. The columns of ϱ encode the structure of the spatial modes of the sub-system.

---

[1] $S_L = \sum_{k=1}^{L} f(d_k)$, where $f(x) = -\left(\frac{1-x}{2}\right)\log\left(\frac{1-x}{2}\right) - \left(\frac{1+x}{2}\right)\log\left(\frac{1+x}{2}\right)$.

35

4.1.1 CRITICAL XY MODEL

Here we present the entropy of entanglement S_L for two different critical regimes and show that the manifestation of this criticallity is in the scaling behavior of the entropy as a function of L.

In fig.(4.1.1) we show the entanglement entropy S_L as a function of sub-system size L in the critical region where $\gamma = 0$. We see that this plot perfectly fits a logarithmic behavior of the form

$$S_L = \frac{1}{3} \log L + c_1 \tag{4.1}$$

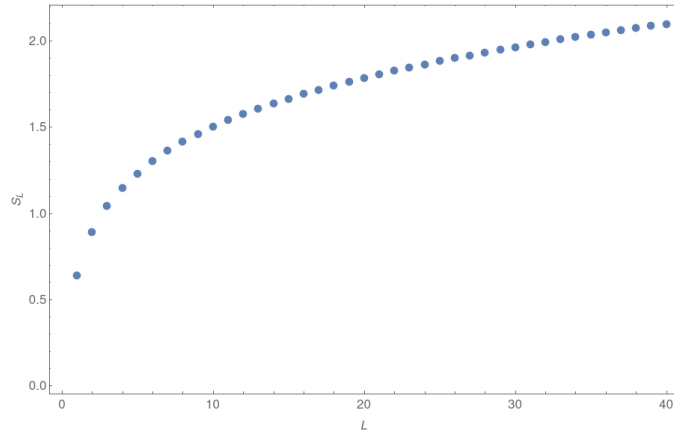as predicted by conformal theory [for further details see [16, 30]].

Figure 4.1.1: Entanglement entropy S_L as a function of sub-system size L for the parameters $\gamma \to 0$ and $\lambda = 1/2$ in a spin chain of $N = 401$ sites.

On the other hand fig.(4.1.2) shows the entanglement entropy S_L as a function of sub-system size L in the critical region where $\lambda = 1$. Again, it perfectly fits a logarithmic behavior of the form
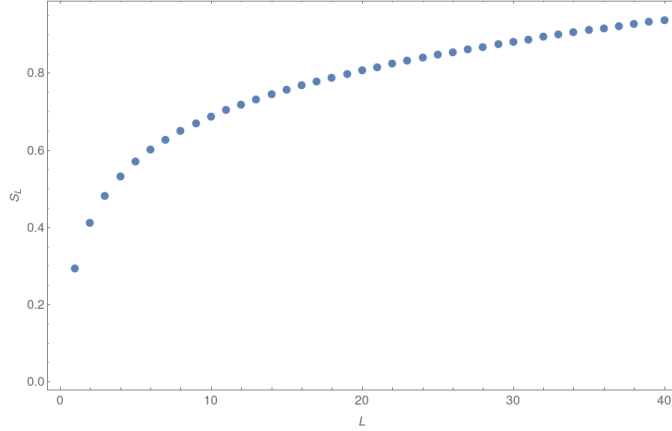
$$S_L = \frac{1}{6} \log L + c_2 \tag{4.2}$$

Figure 4.1.2: Entanglement entropy S_L as a function of sub-system size L for the parameters $\gamma = 1/3$ and $\lambda \to 1$ in a spin chain of $N = 401$ sites.

as predicted by conformal theory [16, 30].

4.1.2 AREA LAW FOR THE ENTROPY OF ENTANGLEMENT

The 1-dimensional version of area law is presented in fig.(4.1.3), where we note that S_L saturates to a constant value. Remember that the *area law scaling* behavior of S_L says that this quantity grows merely with the size of the boundary of the block, then this saturation makes sense since the boundary of a 1D region is just the two endpoints of the block.

Computing the participation function ϱ we see that the locality in the quantum correlation is manifest also in the shape of this matrix. The first important feature in fig.(4.1.4) is that the columns in ϱ, representing the spatial modes for the block are somehow localized but more importantly the only mode that contributes to the entanglement is the one localized at the very ends of the block. This is evident in fig.(4.1.5) where we see that only one mode contributes with a term of
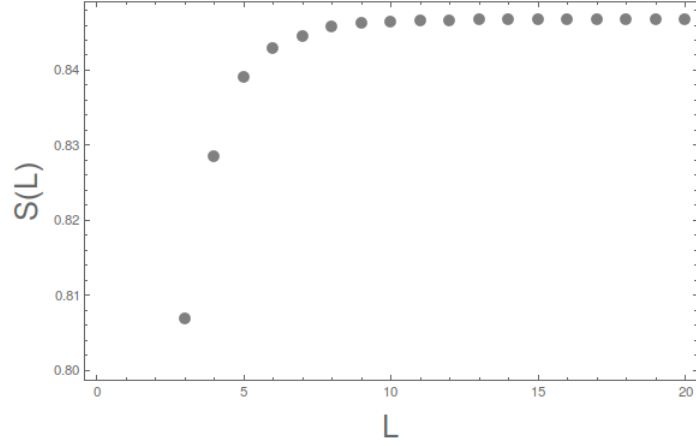
Figure 4.1.3: Entanglement entropy S_L as a function of sub-system size L for the parameters $\gamma = 0.3$ and $\lambda = 0.6$ in a spin chain of $N = 200$ sites.
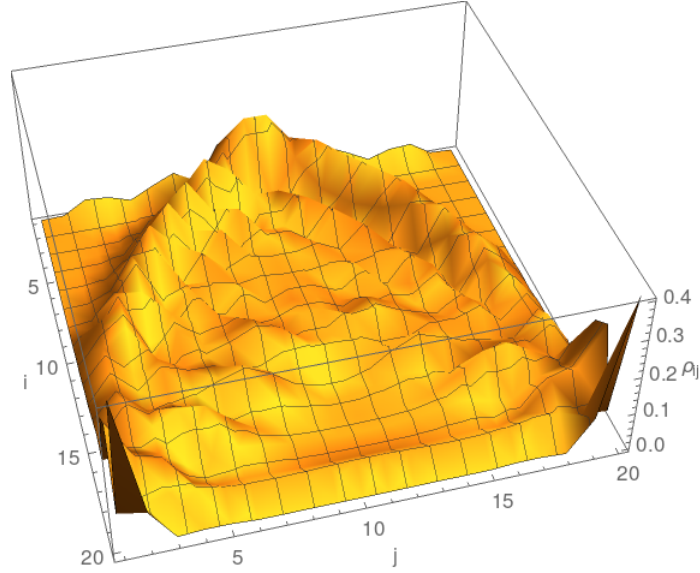

Figure 4.1.4: Participation function for the parameters $\gamma = 0.3$ and $\lambda = 0.6$ in a spin chain of $N = 200$ sites and a block of $L = 20$ adjacent spins.

order $\mathcal{O}(1)$ to the entropy.

This is in good agreement with the exponential decay of correlations present in this model away from critical points.
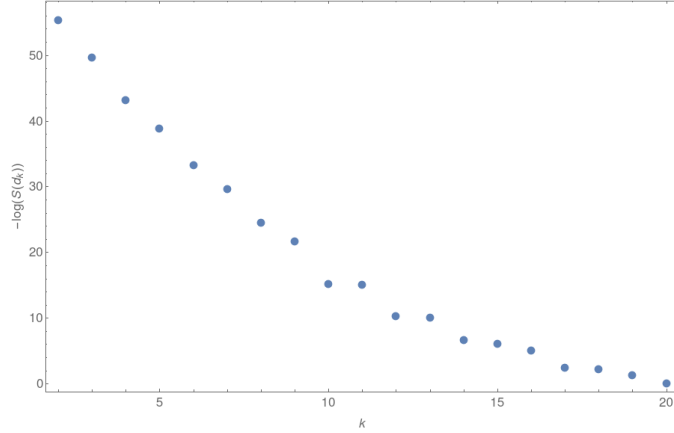
Figure 4.1.5: Logarithmic plot of the individual contribution to the entropy $S(\lambda_k)$ as a function of the mode k for the parameters $\gamma = 0.3$ and $\lambda = 0.6$ in a spin chain of $N = 200$ sites and a block of $L = 20$ adjacent spins.

4.2 MACROSCOPICALLY EXCITED STATES AND THERMAL STATES

Thermal states of the XY model are understood as averages of individual instances of macroscopically excited states (MES) generated at a certain temperature β. Each MES is defined by the set of occupation numbers for the modes labeled by k and is generated from the Fermi-Dirac distribution in (3.37).

4.2.1 VOLUME LAW FOR ENTANGLEMENT ENTROPY IN MACROSCOPICALLY EXCITED STATES

In fig.(4.2.1) we plot the entropy S_L as a function of the block size, L, for a MES at non-zero temperature. In contrast to the *area law* for ground state here we have that the entropy scales linearly with the block size, which is a *volume law* in the entanglement entropy. Even though we show this results just for one particular MES state this behavior is
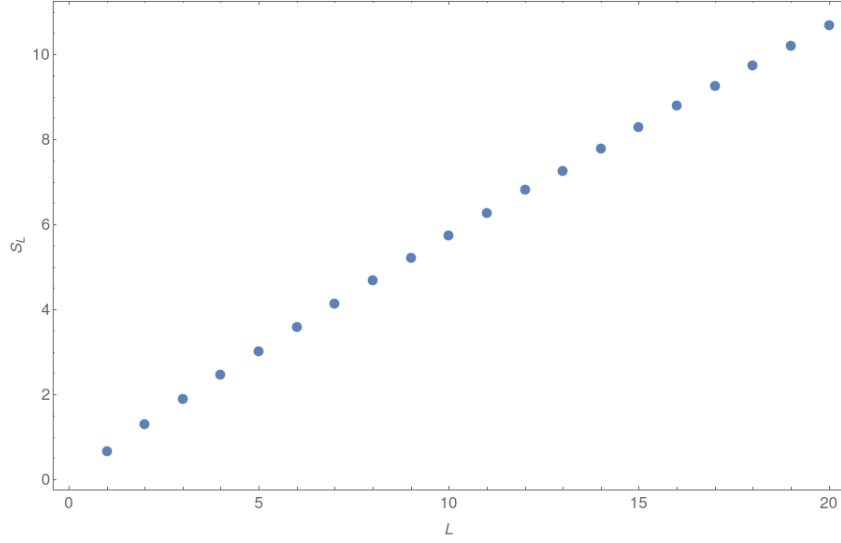
39

Figure 4.2.1: S_L as a function of the mode L for the parameters $\gamma = 0.3$ and $\lambda = 0.6$ at inverse temperature β in a spin chain of $N = 200$.
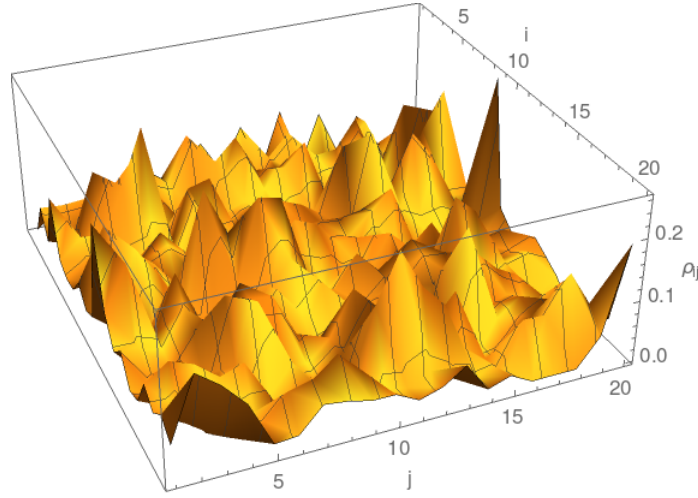

Figure 4.2.2: Participation function for the parameters $\gamma = 0.3$ and $\lambda = 0.6$ in a MES at temperature β for $N = 200$ sites and a block of $L = 20$ adjacent spins.

presented in every MES state generated.

Analogously to the ground state we compute the participation func-

tion for this particular MES state. We see from fig.(4.2.2) that the participation function does not show a particular spatial structure. Every mode is entangled with the rest of the modes which is consistent with the fact that every normal mode contributes with a term of order $\mathcal{O}(1)$ to the entanglement as shown in fig.(4.2.3). We emphasize that the
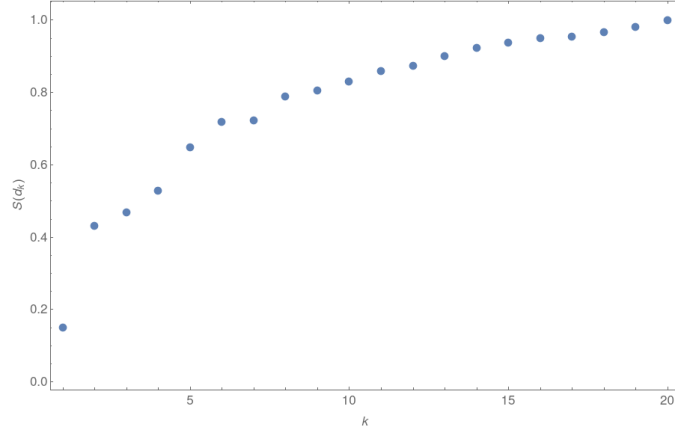

Figure 4.2.3: Individual contribution to the entropy $S(\lambda_k)$ as a function of the mode k for a MES at temperature $\beta = 1$ for the parameters $\gamma = 0.3$ and $\lambda = 0.6$ in a spin chain of $N = 200$ sites and a block of $L = 20$ adjacent spins.

volume law scaling of the entropy of entanglement is present for any MES generated from the fermionic occupation numbers. None of these MES can have exponential decay of correlations but thermal states.

4.2.2 PRINCIPAL COMPONENT ANALYSIS FOR THE FCM OF THERMAL STATES

Generating a sufficient amount of MES at a given temperature, β, one can approximate thermal states as the average of this individual instances. For generating reduced FCM of thermal states we do the following (every MES is generated a the same β):

- Sample from the Fermi-Dirac distribution (3.37) the 'cosine' and 'sine' occupation numbers, $n^c(\theta_k)$ and $n^s(\theta_k)$ respectively, for each mode labeled by k. This we call Gibbs sampling.

- Generate the bands (antibands) for matrices M^+ and M^- in position space.

- Take the $L \times L$ sub-matrix of M^+ and M^-. Note that this correspond to take $2L - 1$ different values (bands or antibands) in each matrix.

- Store them in a $(4L-2)-$dimensional vector (we will refer to this vector as the FCM of the particular MES).

- Repeat D times.

Now we end up with a 'cloud' of D vectors in a $(4L - 2)-$dimensional space that we will call the data set. As stated before, even though each vector representing the reduced FCM for the block of L spins does not fulfill exponential decay of correlations, the resulting state does. The fluctuations given by the individual contributions of each MES are responsible for the resulting exponentially decaying signal in the correlation functions, thus we perform a PCA on the D vectors to study the fluctuations around the mean FCM. In fig.(4.2.4) we show the eigenvalues of the correlation matrix generated with the FCMs. This eigenvalues express the ratio between the variation explained by each principal component and the total variation of the data set. The first thing we notice is that there are $L - 1 = 17$ eigenvalues that are zero. These zero eigenvalues comes from the circulant sector of the fluctuations in the FCM.

Fig.(4.2.5) shows numerically what we found in (3.50). The first $L = 18$ points represent approximately the eigenvectors $\boldsymbol{c}(\theta_i)$ of the
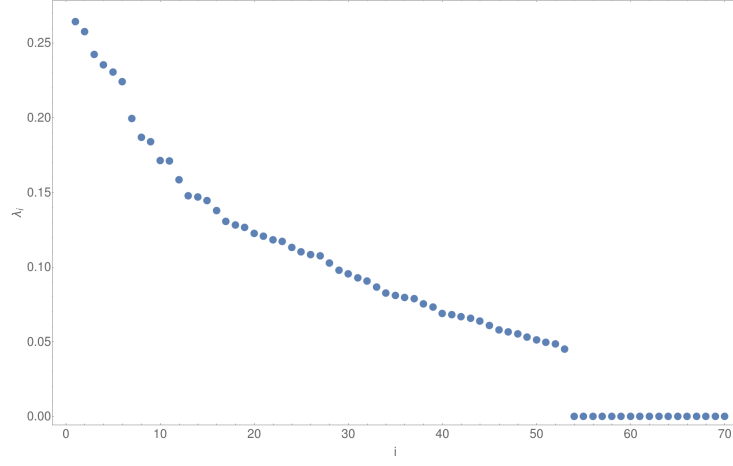
Figure 4.2.4: Eigenvalues of the correlation matrix of the data set for $\gamma = 0.3$ and $\lambda = 0.6$ in a at temperature $\beta = 1$ for $N = 201$ sites and a block of $L = 18$ adjacent sites.
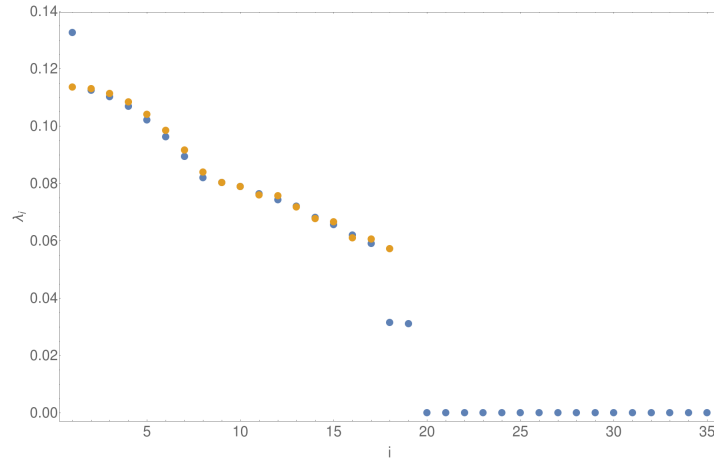

Figure 4.2.5: (Blue) Eigenvalues of the correlation matrix of the data corresponding the the circulant part of M. (Orange) $\nu(\theta_i)(1 - \nu(\theta_i))/2$ as a function of i, where $\theta_i = 2\pi i/(2L - 1)$. Parameters: $\gamma = 0.3$, $\lambda = 0.6$, $\beta = 1$, $N = 201$ and $L = 18$.

matrix $B^{(L)}$ with eigenvalue, $\nu(\theta_i)(1 - \nu(\theta_i))/2$, given the fit between the two plots. This correspondence shows that the most fluctuating modes are low-frequency modes since the maximum the eigenvalue is

reached when $\nu(\theta_i) = 1/2$.

The $(L+1)-$th eigenvalue correspond to the vector $\boldsymbol{r}$ where all the remaining $L-1$ vectors $\boldsymbol{s}(\theta_i)$ are mapped by this $B^{(L)}$. In summary, the $(2L-1) \times (2L-1)$ matrix $B^{(L)}$ has rank $L+1$ and its eigenvectors are approximately the vectors $\boldsymbol{c}(\theta_i)$, whose components are defined in (3.43), for $i = 0, 1, \ldots, L$. The remaining $2L-1$ eigenvalues in fig.(4.2.4) come from the anticirculant sector of the fluctuations of the FCM.

Since $B^{(L)}$ is a banded matrix, its eigenvectors are also banded matrices. In fig.(4.2.6) we plot the bands of the first $L+1 = 19$ eigenvectors corresponding to the non-zero eigenvalues in fig.(4.2.5).
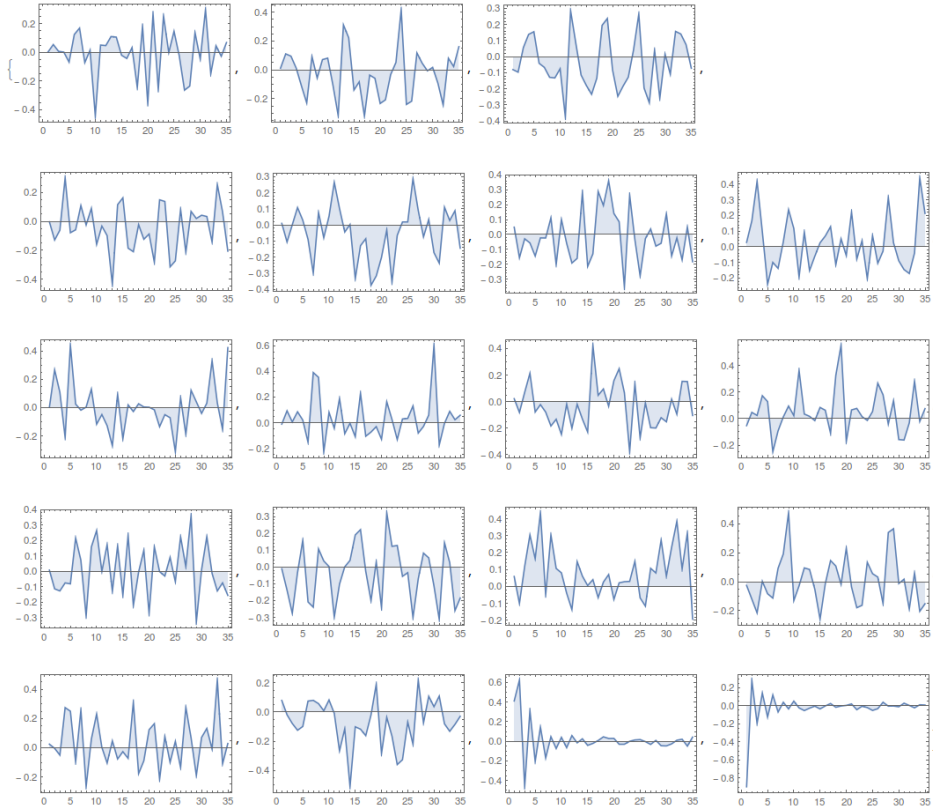

Figure 4.2.6: Plot of the $2L-1$ bands of the first $L+1 = 19$ eigenvectors of the correlation matrix of the data for $\gamma = 0.3$, $\lambda = 0.6$ and $N = 201$.

We may think the PCA as a method to purpose a statistical model for the fluctuations in the FCM. A possible solution is to think that a the matrix F, representing the fluctuations around the mean covariance matrix is generated as

$$F = \frac{1}{n_{\max}} \sum_{i=1}^{n_{\max}} w_i M_i \qquad (4.3)$$

where $n_{\max}$ is the number of eigenvectors (called principal components) used to represent F, M_i are the eigenvectors of the correlation matrix and w_i are coefficients sampled from normal distributions $N(0, \lambda_i)$; with λ_i the eigenvalues in fig.(4.2.5). The model in (4.3) may be useful when the number of principal components that explain a high percent of the total variation since it provides a complexity reduction to the problem. Here we observe that the number of principal components for the fluctuation matrix are not few. Therefore the fluctuation matrix is composed of several principal components, each modulated by quantities of the same order. In fig.(4.2.7) we plot the intensities[2] of the bands as a function of distance δ from the diagonal, for each principal component.

Even though a decaying shape is observed for the intensity as a function of δ for almost every principal component, all these values are of the same order. In conclusion, the fact that the eigenvalues of the correlation matrix for the FCM are comparable to each other, together with the intensities of the bands being also of the same order between them, may explain that cancellations of individual contributions to the correlation functions occur when summing to obtain the FCM of a thermal state, which exhibits exponential decay of correlations.

We have shown the results only for $\gamma = 0.3$ and $\lambda = 0.6$ but the qual-

---

[2]The intensity is computed as the root mean square of the two bands that are δ away from the central band.
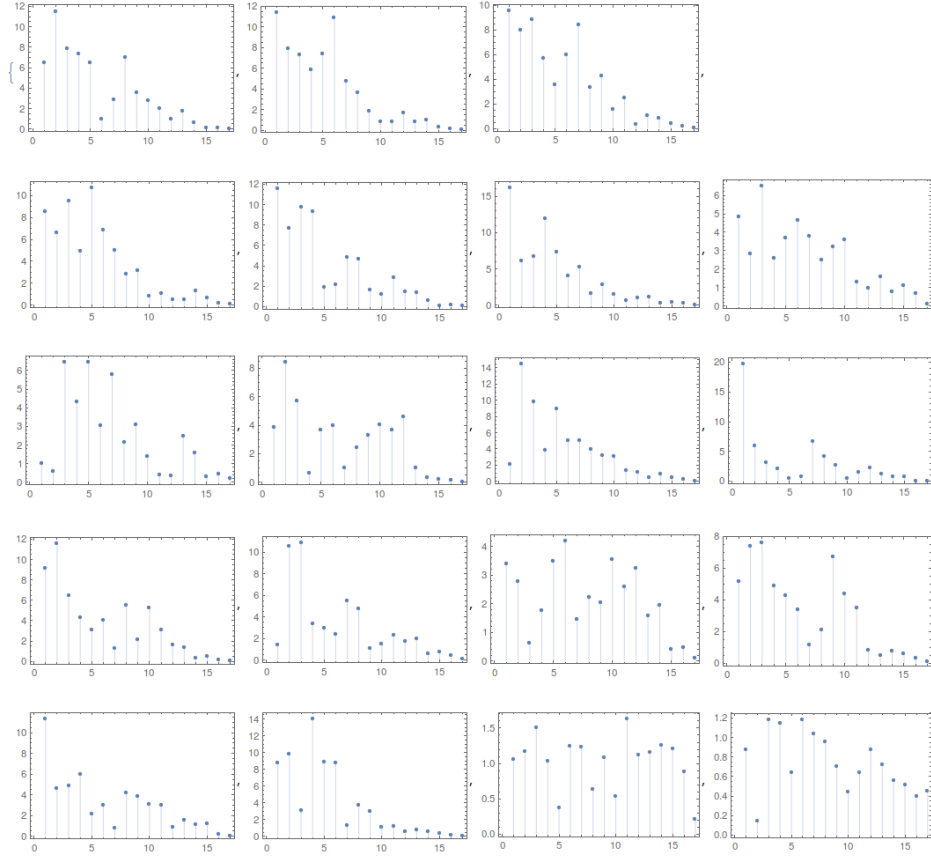
Figure 4.2.7: Intensity of a band as a function of 'band distance' δ for the $L + 1 = 19$ eigenvectors of the correlation matrix.

itative results discussed here are robust for a big set of the parameters of the model as long as we are away from critical regions.

5

Conclussion and Outlook

We have used the fact that all eigenstates of the XY model are completely characterized by its fermionic covariance matrix and canonical typicallity arguments to study the problem of the scaling nature of correlation functions for thermal states understood as averages over eigenstates of the XY Hamiltonian describing a given number of quasi-particle excitations. Each state constituting a thermal state is, with very high probability, maximally entangled, therefore does not fulfill *area law* and consequently do not have exponential decay of correlations. But after the average over macroscopically excited states, somehow the fluctuations around the mean signal on the correlation functions cancel resulting in an exponential decaying signal for the thermal states. These fluctuations around the mean fermionic covariance matrix for sub-systems of the XY model can always be expressed as a sum

of a banded matrix and an antibanded matrix.

For the ground state of the XY model we explored the information stored in the spatial modes about the entanglement entropy. In critical regions the scaling of the entanglement entropy with the sub-system size, L, fits perfectly a logarithmic behavior as predicted by conformal field theory. In the case of non-critical regimes the *area law* is manifested in the fact that the entropy of entanglement saturates to a constant value since the boundary region of a 1D sub-chain is just the two endpoints. The spatial modes show that individual contributions of each mode to the entropy decay exponentially. In practice, the entropy of entanglement is due to just one mode (the one localized on the endpoints of the sub-chain).

Performing a principal component analysis to the ensemble of fermionic covariance matrices of eigenstates of the Hamiltonian, at a given temperature, showed that there is a dimensionality reduction since $L - 2$ eigenvalues of the correlation matrix are zero. The circulant sector of the fluctuations of the coviariance matrices corresponds to a rank $L + 1$ matrix whose first L eigenvectors correspond to the Einstein's formula for the fluctuations in the average occupation number and the remaining $L - 1$ are all mapped to a single vector. The fact that these eigenvalues correspond to the fluctuations on the average occupation number tell us that the modes that fluctuate more are modes of low frequency. Also, the fact that the eigenvalues of the correlation matrix for the FCM are comparable to each other, together with the intensity shape for different bands in the principal components, could explain that even though each MES constituting the thermal state does not exhibit exponential decay of correlations, once the summation is done cancellations of individual contributions to the correlation functions occur and it results in an exponentially decaying signal in quantum correlations.

References

[1] M. B. Plenio, J. Hartley, and J. Eisert. Dynamics and manipulation of entanglement in coupled harmonic systems with many degrees of freedom. *New Journal of Physics*, 6(1):36, 2004.

[2] K. Audenaert, J. Eisert, M. B. Plenio, and R. F. Werner. Entanglement properties of the harmonic chain. *Physical Review A*, 66(4):042327, 2002-10-30.

[3] F. Verstraete and J. I. Cirac. Valence-bond states for quantum computation. *Physical Review A*, 70(6):060302, 2004-12-14.

[4] Patrik Recher and Daniel Loss. Dynamical coulomb blockade and spin-entangled electrons. *Physical Review Letters*, 91(26):267003, 2003-12-30.

[5] Daniel Loss and David P. DiVincenzo. Quantum computation with quantum dots. *Physical Review A*, 57(1):120–126, 1998-01-01.

[6] S. Bravyi. Lieb-robinson bounds and the generation of correlations and topological quantum order. *Physical Review Letters*, 97(5), 2006.

[7] Matthew B. Hastings and Tohru Koma. Spectral gap and exponential decay of correlations. *Communications in Mathematical Physics*, 265(3):781–804, 2006-08-01.

[8] Bruno Nachtergaele and Robert Sims. Much ado about something: Why lieb-robinson bounds are useful. *arXiv:1102.0835 [math-ph]*, 2011-02-03.

[9] M. B. Hastings. Lieb-schultz-mattis in higher dimensions. *Physical Review B*, 69(10):104431, 2004-03-29.

[10] Fernando G. S. L. Brandão and Michał Horodecki. Exponential decay of correlations implies area law. *Communications in Mathematical Physics*, 333(2):761–798, 2015-01-01.

[11] J. Eisert, M. Cramer, and M. B. Plenio. Colloquium: Area laws for the entanglement entropy. *Reviews of Modern Physics*, 82(1):277–306, 2010-02-04.

[12] Sandu Popescu, Anthony J. Short, and Andreas Winter. Entanglement and the foundations of statistical mechanics. *Nature Physics*, 2(11):754–758, 2006-11.

[13] Elliott Lieb, Theodore Schultz, and Daniel Mattis. Two soluble models of an antiferromagnetic chain. *Annals of Physics*, 16(3):407–466, 1961-12-01.

[14] Eytan Barouch, Barry M. McCoy, and Max Dresden. Statistical mechanics of the xy model. i. *Physical Review A*, 2(3):1075–1092, 1970-09-01.

[15] Eytan Barouch and Barry M. McCoy. Statistical mechanics of the xy model. II. spin-correlation functions. *Physical Review A*, 3(2):786–804, 1971-02-01.

[16] J. I. Latorre, E. Rico, and G. Vidal. Ground state entanglement in quantum spin chains. *Quantum Info. Comput.*, 4(1):48–92, 2004-01.

[17] Alonso Botero and Benni Reznik. BCS-like modewise entanglement of fermion gaussian states. *Physics Letters A*, 331(1):39–44, 2004-10-11.

[18] Eduardo Fradkin. *Field Theories Of Condensed Matter Systems Vol#82 On-demand Printing Of #52253*. CRC Press, 1 edition edition, 1997-08-06.

[19] E. Greplová. *Quantum Information with Fermionic Gaussian States*, master thesis, 2013.

[20] J. S. Calderón-García and A. F. Reyes-Lega. Majorana fermions and orthogonal complex structures. *Modern Physics Letters A*, 33(14):1840001, 2018-05-08.

[21] Christina V. Kraus, Michael M. Wolf, J. Ignacio Cirac, and Géza Giedke. Pairing in fermionic systems: A quantum-information perspective. *Physical Review A*, 79(1):012306, 2009-01-08.

[22] Charles H. Bennett, Herbert J. Bernstein, Sandu Popescu, and Benjamin Schumacher. Concentrating partial entanglement by local operations. *Physical Review A*, 53(4):2046–2052, 1996-04-01.

[23] Ryszard Horodecki, Paweł Horodecki, Michał Horodecki, and Karol Horodecki. Quantum entanglement. *Reviews of Modern Physics*, 81(2):865–942, 2009-06-17.

[24] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev. Entanglement in quantum critical phenomena. *Physical Review Letters*, 90(22):227902, 2003-06-02.

[25] Itai Arad, Zeph Landau, and Umesh Vazirani. Improved one-dimensional area law for frustration-free systems. *Physical Review B*, 85(19):195145, 2012-05-29.

[26] H. Bernigau, M. J. Kastoryano, and J. Eisert. Mutual information area laws for thermal free fermions. *Journal of Statistical Mechanics: Theory and Experiment*, 2015(2):P02008, 2015.

[27] Michael M. Wolf, Frank Verstraete, Matthew B. Hastings, and J. Ignacio Cirac. Area laws in quantum systems: Mutual information and correlations. *Physical Review Letters*, 100(7):070502, 2008-02-20.

[28] Shigetoshi Katsura. Statistical mechanics of the anisotropic linear heisenberg model. *Physical Review*, 127(5):1508–1518, 1962-09-01.

[29] Yuezhen Niu, Suk Bum Chung, Chen-Hsuan Hsu, Ipsita Mandal, S. Raghu, and Sudip Chakravarty. Majorana zero modes in a quantum ising chain with longer-ranged interactions. *Phys. Rev. B*, 85:035110, Jan 2012.

[30] Curtin Callan and Frank Wilczek. On geometric entropy. *Physics Letters B*, 333(1):55–61, 1994-07.