UNIVERSIDAD DE LOS ANDES

MASTER'S THESIS

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

Author:
Mario HENAO-AYALA

Supervisor:
Dr. Alonso BOTERO

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Declaration of Authorship

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Abstract

Faculty Name
Department of Physics

Master in Science - Physics

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

by Mario HENAO-AYALA

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

Acknowledgements

The acknowledgments and the people to thank go here, don't forget to include your project advisor…

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List of Abbreviations

LAH	**L**ist **A**bbreviations **H**ere
WSF	**W**hat (it) **S**tands **F**or

Physical Constants

Speed of Light $c_0 = 2.997\,924\,58 \times 10^{8}\,\mathrm{m\,s^{-1}}$ (exact)

List of Symbols

a	distance	m
P	power	W ($J\,s^{-1}$)
ω	angular frequency	rad

For/Dedicated to/To my…

Chapter 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 [cite:introBCSlike]. Additionally, entanglement has applications in diverse quantum computation tasks [cite:introBCSlike].

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 (i.e. ground states) 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 functions.

On the other hand, the study of correlation functions [comment on corr. func.] 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:

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

where O_A and O_B are operators acting in the subspaces 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.

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 [cite:correlations-arealaws] about the relation of these two quantities.

In year Hastings et al. [cite:Hastings.ref4.Brandao] showed that in any dimensions, the ground state of a gapped Hamiltonian always present exponential decay of correlations.

The XY model was introduced first by Lieb, Schultz and Mattis [cite:LMS2SolvMod] to study the influence of symmetry in many-body systems. It represents a set of spin-$1/2$ particles in a $D-$dimensional lattice where each particle interacts only with its nearest neighboring sites and an external magnetic field. This spin-chain system can be mapped, via a Jordan-Wigner transformation, to a quadratic Hamiltonian in fermionic operators.

In 1970 Barouch and McCoy [cite:StatMechXYmodel2] 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.

Chapter 2

Theoretical background

In this chapter we introduce the concepts of free fermionic models on a lattice...

2.1 Fermionic quadratic Hamiltonians

In many-body physics, there are many models that 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

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

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

$$\{b_i^{\dagger}, b_j^{\dagger}\} = \{b_i, b_j\} = 0, \quad \{b_i^{\dagger}, b_j\} = \delta_{ij}, \tag{2.2}$$

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

Important classes of models that are described in terms of Hamiltonians like (2.1) are Hubbard models [referencia], the BCS theory of superconductivity in the *mean field* approximation [referencia] and spin chains after a Jordan-Wigner transformation (which is the most relevant class for this work) [LatorreVidal,12introBCS]. Hamiltonians of the generic form of (2.1) are diagonalized through Bogoliubov transformations (i.e., canonical transformations). These transformations map interacting fermions into non-interacting quasi-particles (fermions) that are expressible as a linear combination of the creation and annihilation operators b, $b^{\dagger}$, that is,

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

where u_i^j and u_i^j are complex numbers restricted due to 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 farctorize as stated in Wick's theorem [master thesis Greplova]. 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 *Clifford algebra*[1]. Changing from fermions described by the vector of fermionic operators $b^T := (b_1, b_2, \dots, b_N, b_1^\dagger, b_2^\dagger, \dots, b_N^\dagger)$ to the vector of Majorana operators $\gamma^T := (\gamma_1, \gamma_2, \dots, \gamma_N, \gamma_{1+N}, \gamma_{2+N}, \dots, \gamma_{2N})$ is often convenient to define the *fermionic covariance matrix* which completely specifies *fermionic gaussian states*.

2.1.2 Fermionic Gaussian States and Fermionic Covariance Matrix

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

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

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

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

where $\tilde{B} = diag(\tilde{\beta}_k)$ and $O \in O(2N)$. The right hand side of (2.7) is known as the Williamson form of the anti-symmetric 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

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

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

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

where the $\lambda_k = \tanh(\beta_k/2)$ for $k = 1, \dots, N$ [Kraus-Pairing ferm sys] which determines the connection between the matrix G in (2.6) and the *fermionic covariance 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 quasi-particle excitations.

[1]The orthogonal group in $2N$ dimensions $O(2N)$ preserves the *Clifford algebra* hence the canonical anti-commutation relations of fermionic operators.

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 anti-commutation 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 [Latorre].

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. [Bennett concentrating partial ent...]. 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 [ref sobre LOCC]. 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 $S(\rho)$ [Latorre]. The entanglement entropy makes sense only after a bipartition of the full system and is the von Neumann entropy of the reduced density matrix $\rho_A := \operatorname{tr}_B \rho$, where tr_B means tracing out the degrees of freedom of the complementary system B

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

of the subsystem A, that is,

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

The results obtained in the literare 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. [Vidal - ent in quan crit phen] to explore the behavior of quantum correlations at different length scales dictated by the size, L, of the block (subsystem) 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

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

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.(**??**) we depict the situation stated above.

figure

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 make up the chain. This extensive behavior is referred as *volume law scaling* of entanglement entropy observed in thermal states [mutual inf area law, eisert-colloquium]. 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*[Hastings...] because it is merely linear with the size of the boundary of the block of L sites.

figure area law

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 [eisert - colloquim]]. 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 [brandao horodecki].

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 typicality

The following results are discused in detail in the work of Popescu, Short and Winter [popescu can typ]. 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 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, of the state consistent with the restriction, R, correspond to 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 i.e. it represents that the total energy of the *universe* is close to a given number ε. Thus almost avery pure state on the *universe* is such that the *system* is in the thermal canonical state

$$\Omega_S^{(\varepsilon)} \propto \exp[-\beta H_S], \tag{2.15}$$

[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.

where H_S is the Hamiltonian of the *system* and 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 [Popescu...].

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 generla class of fermionic gaussian states.

Due to canonical typicality arguments the random pure states drawn from the Haar 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 [brandao horodecki] tell us that if a state has entanglement entropy that fulfills *volume law* 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

$$\rho = \sum_\alpha p_\alpha \left|\Phi_\alpha\right\rangle \left\langle\Phi_\alpha\right| . \tag{2.16}$$

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 no 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(s) contribution to result in 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 for 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.

Chapter 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. These results are a review of previous works in spin chains. The first exact solution for the XY model, for magnetic field $\lambda = 0$, was presented by Lieb, Schultz and Mattis [LSM]. Then Katsura [katsura - stat mech of the heisenberg] 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 ent in quan crit phen] we mention some basic aspects on the criticallity of this model [see [latorre] for further details].

3.1 The XY Hamiltonian

The XY Hamiltonian models a set of N spin-1/2 particles located on the sites of, in principle, 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

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

here γ is the anisotropy parameter and represents the difference between the strength of the $x-$interaction and the $y-$interaction (in spin space) and λ is the intensity of the external magnetic field. On the other hand

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

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

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

figure spin chain

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. (ii) For $\gamma = 1$ (3.1) corresponds to the Ising model. (iii) The Kitaev chain is equivalent to the XY model under an proper identification of the parameters μ, t and Δ with γ and λ.

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 anti-commutation 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 anti-commmutation 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 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 anti-commutation 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

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

and with this transformation the Hailtonian takes the diagonal form

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

with

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

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

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

3.1.2 The XY model in the $(\gamma, \lambda)-$plane

We can use the expression (3.13) for the spectrum to identify regions in the $(\gamma, \lambda)-$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

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

Near critical points, this correlation length diverges when the model approaches the critical value of the magnetic field λ. Distinct behaviors are present for this divergence, one for $\gamma = 0$ and another for $\gamma = (0, 1]$ [latorre - spin chains, barouch-mccoy]. Barouch and McCoy showed that in the line $\gamma^2 + \lambda^2 = 1$ there is also a divergence in the correlation length. In fig.(**??**) we show the critical regions in the XY model in the parameter space.

figure gamma lambda plane.

These results are important when we show the scaling nature of the entanglement entropy with the size of the block.

3.2 Fermionic Covariance Matrix 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

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

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

Note the tree 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 anti-symmetric matrix of the form

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

where

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

Given that $\Omega^{(0)}$ is a circulant and real matrix, it can be diagonilized by means of a Fourier transformation [circulan matrix], then it can be written in terms o an even function $\omega(\theta_k)$ and an odd function $\phi(\theta_k)$ as

$$\Omega_{nm}^{(0)} = \frac{1}{N} \sum_{\theta_k} \omega(\theta_k) e^{i\phi(\theta_k)} e^{i(m-n)\theta_k} = \frac{2}{N} \sum_{\theta_k=0}^{\pi} \omega(\theta_k) \cos\left((n-m)\theta_k + \phi(\theta_k)\right). \tag{3.22}$$

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

$$u_m^c(\theta_k) = \sqrt{\frac{2}{N}}\cos(m\theta_k + \phi(\theta_k)), \quad u_m^s(\theta_k) = \sqrt{\frac{2}{N}}\sin(m\theta_k + \phi(\theta_k))$$
$$v_m^c(\theta_k) = \sqrt{\frac{2}{N}}\sin(m\theta_k), \quad v_m^s(\theta_k) = \sqrt{\frac{2}{N}}\sin(m\theta_k) \tag{3.23}$$

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

$$\Omega_{nm}^{(0)} = \sum_{\theta_k=0}^{\pi} \omega(\theta_k)[u_m^c(\theta_k)v_n^c(\theta_k) + u_m^s(\theta_k)v_n^s(\theta_k)] \tag{3.24}$$

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

$$H^{(N)} = \sum_{n,m=0}^{N-1} \frac{i}{4} \sum_{\theta_k=0}^{\pi} \omega(\theta_k)[u_m^c(\theta_k)v_n^c(\theta_k) + u_m^s(\theta_k)v_n^s(\theta_k)][\gamma_n, \gamma_{m+N}], \tag{3.25}$$

and rearranging things we get

$$H^{(N)} = \frac{i}{4} \sum_{\theta_k=0}^{\pi} \omega(\theta_k)(\underbrace{[\gamma_k^c, \gamma_{k+N}^c]}_{1-2\sigma_k^z} + \underbrace{[\gamma_k^s, \gamma_{k+N}^s]}_{1-2\sigma_k^z}), \tag{3.26}$$

where

$$\gamma_k^{c,s} := \sum_n u_n^{c,s}(\theta_k)\gamma_n, \quad \gamma_{k+N}^{c,s} := \sum_n v_n^{c,s}(\theta_k)\gamma_{n+N}. \tag{3.27}$$

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

$$M_{mn} = \sum_{\theta_k=0}^{\pi} [m^c(\theta_k)u_m^c(\theta_k)v_n^c(\theta_k) + m^s(\theta_k)u_m^c(\theta_k)v_n^c(\theta_k) + m^s(\theta_k)] \tag{3.28}$$

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

$$M_{mn} = \sum_{\theta_k=0}^{\pi} \frac{m^c(\theta_k) + m^s(\theta_k)}{2}(u_m^c(\theta_k)v_n^c(\theta_k) + u_m^s(\theta_k)v_n^c(\theta_k))$$
$$+ \sum_{\theta_k=0}^{\pi} \frac{m^c(\theta_k) - m^s(\theta_k)}{2}(u_m^c(\theta_k)v_n^c(\theta_k) - u_m^s(\theta_k)v_n^c(\theta_k)). \tag{3.29}$$

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 (3.24) to have

$$M_{mn} = \underbrace{\sum_{\theta_k=-\pi}^{\pi} m^+(\theta_k)e^{i\phi(\theta_k)}e^{i(n-m)\theta_k}}_{:=M_{mn}^+} + \underbrace{\sum_{\theta_k=-\pi}^{\pi} m^-(\theta_k)e^{i\phi(\theta_k)}e^{i(n+m)\theta_k}}_{:=M_{mn}^-}. \tag{3.30}$$

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

$$\nu(\theta_k) := \Pr(n^{c,s}(\theta_k) = 1) = \frac{1}{e^{\beta\omega(\theta_k)} + 1}, \tag{3.32}$$

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

$$(\Delta M^\pm)_{mn} = 2\sum_{\theta_k=0}^{\pi} \left(\frac{\Delta n^c(\theta_k) \pm \Delta n^s(\theta_k)}{2}\right) \cos\left((m \mp n)\theta_k + \phi(\theta_k)\right). \tag{3.33}$$

Then the fluctuation matrix has three terms

$$\begin{aligned}\left\langle (\Delta M^\pm)_{mn} \Delta M^\pm)_{m'n'} \right\rangle = \frac{1}{2}\sum_{\theta_k=0}^{\pi} &\left(\left\langle \Delta n^c(\theta_k)^2 \right\rangle + \left\langle \Delta n^s(\theta_k)^2 \right\rangle\right) \times \\ &\times \cos\left((m \mp n)\theta_k + \phi(\theta_k)\right) \cos\left((m' \mp n')\theta_k + \phi(\theta_k)\right),\end{aligned} \tag{3.34}$$

and

$$\begin{aligned}\left\langle (\Delta M^+)_{mn} \Delta M^-)_{m'n'} \right\rangle = \frac{1}{2}\sum_{\theta_k=0}^{\pi} &\left(\left\langle \Delta n^c(\theta_k)^2 \right\rangle - \left\langle \Delta n^s(\theta_k)^2 \right\rangle\right) \times \\ &\times \cos\left((m \mp n)\theta_k + \phi(\theta_k)\right) \cos\left((m' \mp n')\theta_k + \phi(\theta_k)\right),\end{aligned} \tag{3.35}$$

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 anti-circulant matrix we define the anti-band indices $a = m + n$ and $a' = m' + n'$.

[1] An anti-circulant matrix A has the form

$$A = \begin{pmatrix} a_1 & a_2 & \cdots & a_{N-1} & a_N \\ a_2 & a_3 & \cdots & a_N & a_1 \\ \iddots & \iddots & \iddots & \cdots & \iddots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ a_N & a_1 & a_2 & \cdots & a_{N-1} \end{pmatrix} \tag{3.31}$$

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

$$B_{bb'} := \sum_{\theta_k=0}^{\pi} \frac{\nu(\theta_k)(1-\nu(\theta_k))}{2} \cos\left(b\theta_k + \phi(\theta_k)\right) \cos\left(b'\theta_k + \phi(\theta_k)\right), \tag{3.36}$$

and for the anti-circulant matrix

$$A_{aa'} := \sum_{\theta_k=0}^{\pi} \frac{\nu(\theta_k)(1-\nu(\theta_k))}{2} \cos\left(a\theta_k + \phi(\theta_k)\right) \cos\left(a'\theta_k + \phi(\theta_k)\right). \tag{3.37}$$

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

$$\begin{aligned} c_b(\theta_q) &= \cos\left(b\theta_q + \phi_q\right), \quad \text{for } q = 0, 1, \ldots, L-1, \\ s_b(\theta_q) &= \sin\left(b\theta_q + \phi_q\right), \quad \text{for } q = 1, 2, \ldots, L-1. \end{aligned} \tag{3.38}$$

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

$$p(\theta_k) = \frac{\nu(\theta_k)(1-\nu(\theta_k))}{2} \cos\left(b\theta_k + \phi(\theta_k)\right), \tag{3.39}$$

then we have that

$$\sum_{b'} B^{(L)}_{bb'} c_{b'}(\theta_q) = \int_0^{\pi} \frac{d\theta}{2\pi} p(\theta) \sum_{b'} \cos\left(b'\theta + \phi\right) \cos\left(b'\theta_q + \phi_q\right), \tag{3.40}$$

where we have change 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 (3.40) is written as

$$= \frac{1}{2}\int_0^{\pi} \frac{d\theta}{2\pi} p(\theta) \left(\cos\left(\phi + \phi_q\right) \underbrace{\sum_{b'} e^{ib'(\theta+\theta_q)}}_{=D_{L-1}(\theta+\theta_q)} + \cos\left(\phi - \phi_q\right) \underbrace{\sum_{b'} e^{ib'(\theta-\theta_q)}}_{=D_{L-1}(\theta-\theta_q)} \right), \tag{3.41}$$

where

$$D_n(x) := \frac{\sin\left(\left(n+\frac{1}{2}\right)x\right)}{\sin\left(\frac{x}{2}\right)} \tag{3.42}$$

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

$$= \frac{1}{2}\int_{-\pi}^{\pi}\frac{d\theta}{2\pi}p(\theta)\left(\cos\left(\phi+\phi_q\right)D_{L-1}(\theta+\theta_q)+\cos\left(\phi-\phi_q\right)D_{L-1}(\theta-\theta_q)\right) = \tag{3.43}$$

$$\begin{aligned} &= \frac{1}{4}\Bigg(e^{i\phi_q}\overbrace{\sum_{l=-(L-1)}^{L-1} g_l e^{-il\phi_q}}^{\approx g(-\theta_q)} + e^{-i\phi_q}\overbrace{\sum_{l=-(L-1)}^{L-1} h_l e^{-il\phi_q}}^{\approx h(-\theta_q)} \\ &+ e^{-i\phi_q}\underbrace{\sum_{l=-(L-1)}^{L-1} g_l e^{il\phi_q}}_{\approx g(\theta_q)} + e^{i\phi_q}\underbrace{\sum_{l=-(L-1)}^{L-1} h_l e^{il\phi_q}}_{\approx h(\theta_q)}\Bigg) \approx p(\theta_q), \end{aligned} \tag{3.44}$$

where we have used that 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. Also we have used that 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.

In conclusion we have

$$\sum_{b'} B^{(L)}_{bb'} c_{b'}(\theta_q) \approx \frac{\nu(\theta_q)(1-\nu(\theta_q))}{2} c_b(\theta_q), \tag{3.45}$$

which tell us that the vectors $\boldsymbol{c}(\theta_q)$ are approximately eigenvectors of the matrix $B^{(L)}$. This approximation relies on how well are approximated the functions $g(\theta)$ and $h(\theta)$ 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 (3.41) 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.

Finally, it is not possible to treat the matrix $A_{aa'}$, corresponding to the anti-circulant sector of the fluctuations, the same way we did for $B_{bb'}$ since the indices in this case run from 2 to $2L$, and as long as $L \ll N$, which is the case we are always interested, we get no Dirichlet kernels to be able to find analytic solutions.

Chapter 4

Results and Discusion

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

Since every eigenstate of the Hamiltonian (3.1) belong 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.

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

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) 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 [Wilczec, latorre]].

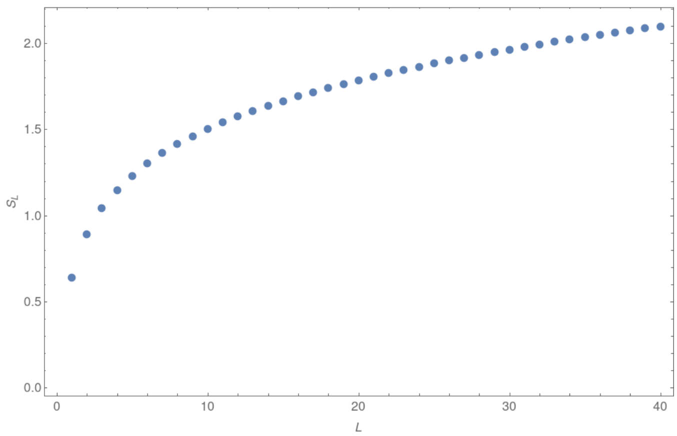

FIGURE 4.1: Entanglement entropy S_L as a function of sub-system size L for the parameters $\gamma \to 0$ and $\lambda = 1/2$ in a spin chain of $N = 401$ sites.

On the other hand fig.(4.2) 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

$$S_L = \frac{1}{6} \log L + c_2 \tag{4.2}$$

as predicted by conformal theory [Wilczec, latorre].

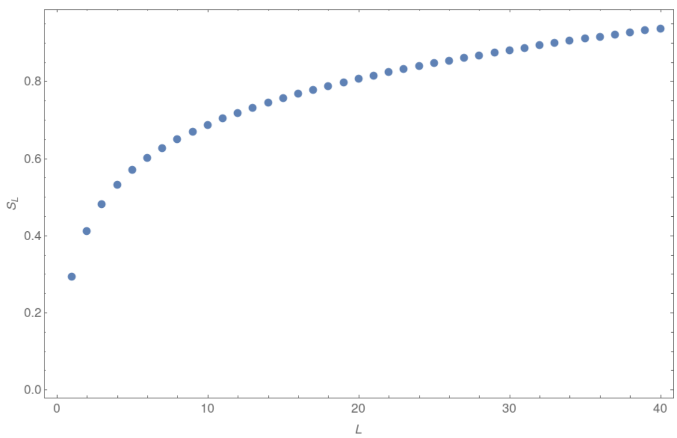

FIGURE 4.2: Entanglement entropy S_L as a function of sub-system size L for the parameters $\gamma = 1/3$ and $\lambda \to 1$ in a spin chain of $N = 401$ sites.

4.1.2 Area law for the entropy of entanglement

The 1-dimensional version of area law is presented in fig.(4.3), 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.

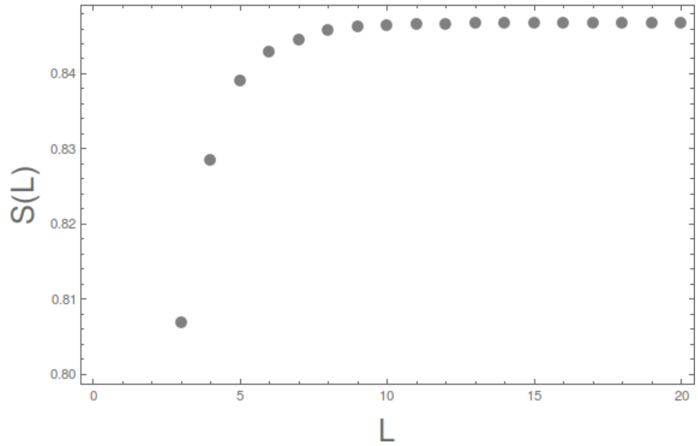

FIGURE 4.3: Entanglement entropy S_L as a function of sub-system size L for the parameters $\gamma = 0.3$ and $\lambda = 0.6$ in a spin chain of $N = 200$ sites.

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

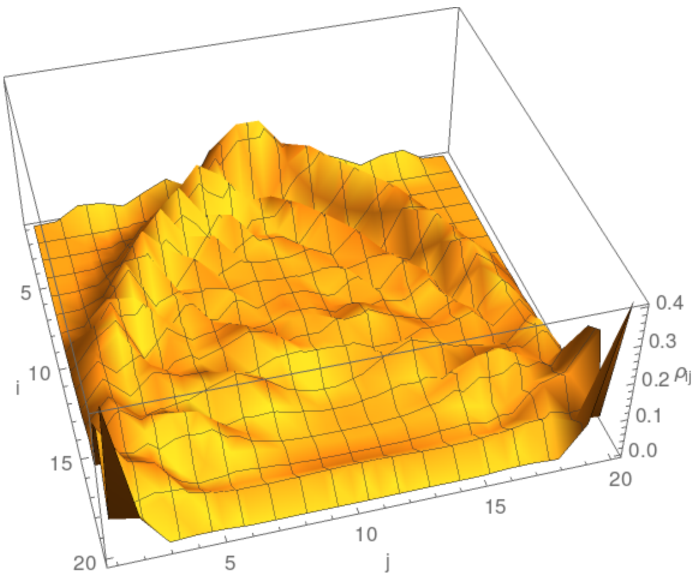

FIGURE 4.4: Participation function for the parameters $\gamma = 0.3$ and $\lambda = 0.6$ in a spin chain of $N = 200$ sites and a block of $L = 20$ adjacent spins.

in fig.(4.4) 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.(4.5) where we see that only one mode contributes with a term of order $\mathcal{O}(1)$ to the entropy.

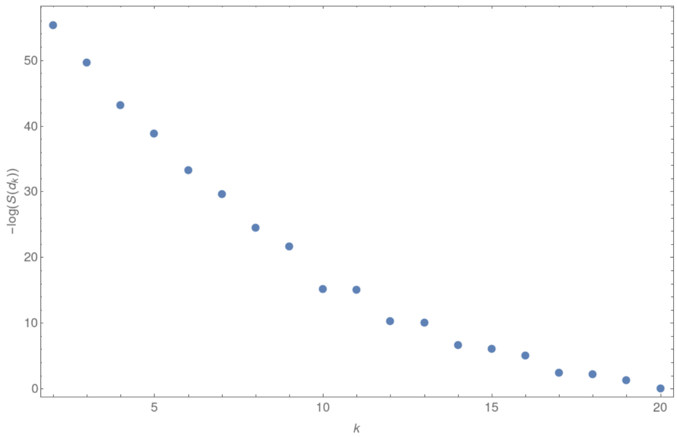

FIGURE 4.5: Logarithmic plot of the individual contribution to the entropy $S(\lambda_k)$ as a function of the mode k for the parameters $\gamma = 0.3$ and $\lambda = 0.6$ in a spin chain of $N = 200$ sites and a block of $L = 20$ adjacent spins.

This is in good agreement with the exponential decay of correlations present in this model away from critical points.

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 (3.32).

4.2.1 Volume law for entanglement entropy in macroscopically excited states

In fig.(4.6) is plotted 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 presented in every MES state generated.

Analogously to the ground state we compute the participation function for this particular MES state. We see from fig.(4.7) 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.(4.8). We emphasize that the *volume law scaling* of the entropy of entanglement is present for any MES generated from the fermionic occupation numbers. Thus each of these MES cannot have exponential decay of correlations but 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):

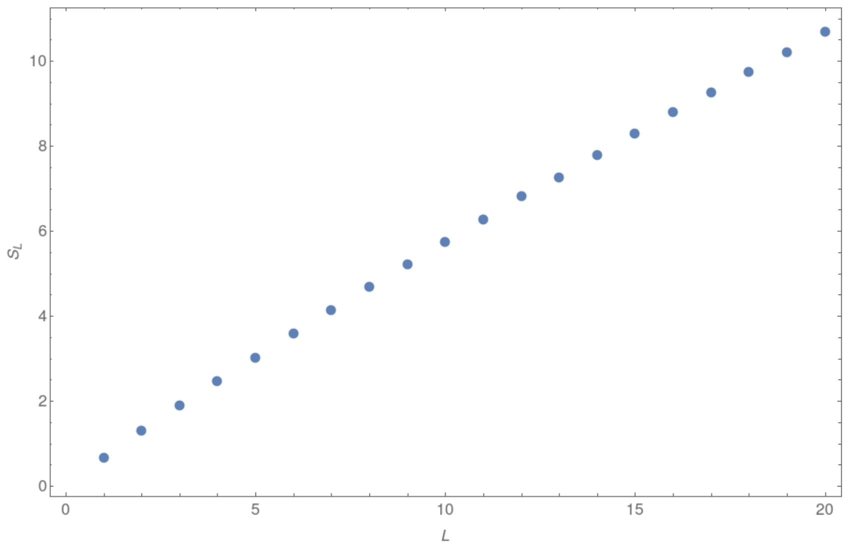

FIGURE 4.6: S_L as a function of the mode L for the parameters $\gamma = 0.3$ and $\lambda = 0.6$ at inverse temperature β in a spin chain of $N = 200$.

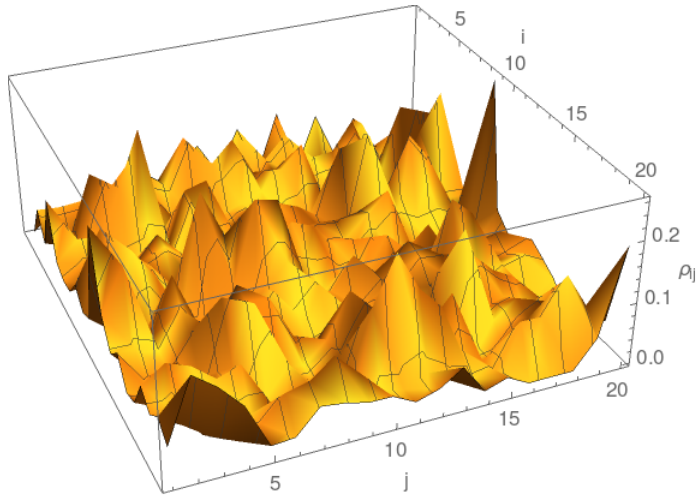

FIGURE 4.7: Participation function for the parameters $\gamma = 0.3$ and $\lambda = 0.6$ in a MES at temperature β for $N = 200$ sites and a block of $L = 20$ adjacent spins.

- Gibbs sample from the Fermi-Dirac distribution (3.32) the 'cosine' and 'sine' occupation numbers, $n^c(\theta_k)$ and $n^s(\theta_k)$ respectively, for each mode labeled by k.
- Generate the bands (anti-bands) 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 anti-bands) in each matrix.
- Store them in a $(4L - 2)-$dimensional vector.
- 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,

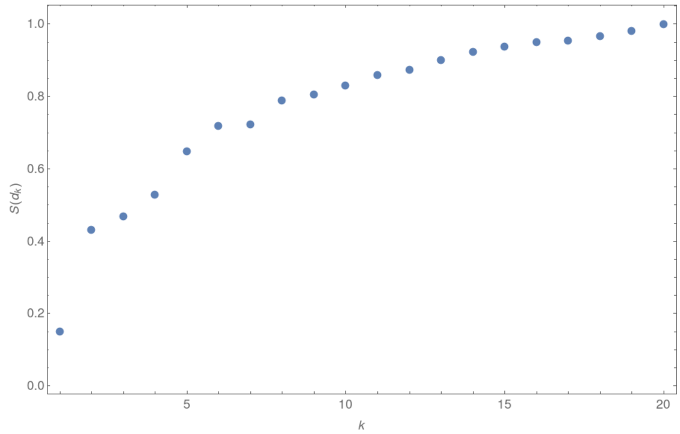

FIGURE 4.8: Individual contribution to the entropy $S(\lambda_k)$ as a function of the mode k for a MES at temperature β for the parameters $\gamma = 0.3$ and $\lambda = 0.6$ in a spin chain of $N = 200$ sites and a block of $L = 20$ adjacent spins.

the resulting state does. The fluctuations given by the individual contributions of each MES are responsible for the resulting exponentially decaying signal. To study this we perform a Principal Component Analysis (PCA) on the D vectors.

The data set is stored in a $D \times (L-1)$ matrix that we call

Appendix A

Frequently Asked Questions

A.1 How do I change the colors of links?

The color of links can be changed to your liking using:
`\hypersetup{urlcolor=red}`, or
`\hypersetup{citecolor=green}`, or
`\hypersetup{allcolor=blue}`.
If you want to completely hide the links, you can use:
`\hypersetup{allcolors=.}`, or even better:
`\hypersetup{hidelinks}`.
If you want to have obvious links in the PDF but not the printed text, use:
`\hypersetup{colorlinks=false}`.