INSTITUTO DE FÍSICA

Universidade Federal Fluminense

Arash Jafarizadeh

Solvable spin and fermionic chains:

A guide to correlations, density matrix formulation and entanglement content

Brasil

30 de agosto de 2022

Arash Jafarizadeh

Solvable spin and fermionic chains:

A guide to correlations, density matrix formulation and entanglement content

"Thesis presented as part of the requirements for obtaining the degree of Doctor of Philosophy by the Physics Institute of Universidade Federal Fluminense."

Universidade Federal Fluminense – UFF

Instituto de Fiśica

Programa de Pós-Graduação

Orientador: Mohammad Ali Rajabpour

Brasil

30 de agosto de 2022

Ficha catalográfica automática - SDC/BIF
Gerada com informações fornecidas pelo autor

J23s Jafarizadeh, Arash
Solvable spin and fermionic chains: A guide to correlations, density matrix formulation and entanglement content / Arash Jafarizadeh ; Mohammad Ali Rajabpour, orientador. Niterói, 2022.
181 f. : il.

Tese (doutorado)-Universidade Federal Fluminense, Niterói, 2022.

DOI: http://dx.doi.org/10.22409/PPGF.2022.d.06508482769

1. Cadeias de spins. 2. Férmions quadráticos. 3. Emaranhamento quântico. 4. Correlação quântica. 5. Produção intelectual. I. Rajabpour, Mohammad Ali, orientador. II. Universidade Federal Fluminense. Instituto de Física. III. Título.

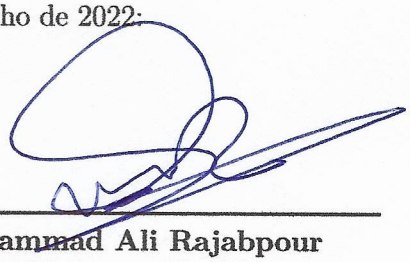
CDD -

Bibliotecário responsável: Debora do Nascimento - CRB7/6368

Arash Jafarizadeh

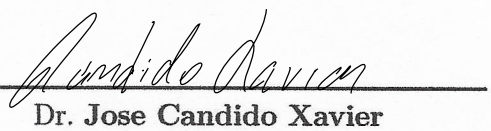
Solvable spin and fermionic chains: A guide to correlations, density matrix formulation, and entanglement content

Trabalho aprovado. Brasil, 15 de julho de 2022:

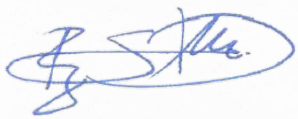


Dr. **Mohammad Ali Rajabpour**
(Orientador)

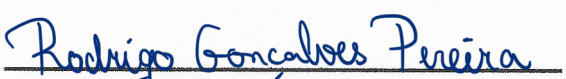
Dr. **Fernando Iemini De Rezende Aguiar**



Dr. **Jose Candido Xavier**



Dr. **Rodrigo Ferreira Sobreiro**



Dr. **Rodrigo Gonçalves Pereira**

Agradecimentos

First, I would like to thank my friends from UFF. To Rafinha, thank you for your friendship and all the support you gave me. To Braian, thank you for all the sharing your worldwide experience involving physics and life, you are a valuable friend. To Davor, thank you for your comedies. Also, I would like thank professor Mercelo Sarandy for his valuable advises, assists and kindness.

To my family, for being such a great parents and supporting me in this journey. Specially to Siavash, I would have not be able to continue in this path without you having my back and holding my hand whenever I was on the edge. I thank Sepanta montazeri for his thoughtful and ironic comments on the life.

Last but not least, thank you Mohammad for sharing with me a huge part of your knowledge during these four years. Since working with you, I have been inspired by your work and wisdom, and I will leave your lab inspired by your research. Although I know that I was not the easiest student you could have, I hope the works compiled here are only the beginning of a fruitful history of scientific collaboration and friendship.

Resumo

As cadeias de spin XY e os modelos de férmions quadráticos relacionados foram amplamente estudados durante os últimos 70 anos atrás. Nesta tese, a solução e a conexão entre o modelo de spin XY solúvel e os férmions quadráticos, obtidos pela fermionização de Jordan-Wigner, são revistos em detalhes. A família de cadeias de spin XY, como a cadeia quântica de Ising e a cadeia de spin XX, tem sido uma grande parte da física quântica de muitos corpos e da informação quântica. Após apresentar a solução para a diagonalização da cadeia de spins XY e o modelo fermiônico, são apresentados outros métodos de formulação de autoestados desses sistemas. Também discuto o conteúdo da função de correlação desses modelos, e não se limita apenas ao estado fundamental. Diferentes formulações do operador de matriz de densidade também são apresentadas da maneira mais abrangente. Todas as quantidades mencionadas são então usadas para estudar o emaranhamento bipartido desses modos. A segunda parte da tese (parte de artigos publicados) contém as aplicações dos métodos fornecidos nas partes anteriores para estudar particularmente o emaranhamento nesta família de modelos. Por exemplo, estudamos a média do emaranhamento de subsistemas em modelos fermiônicos gerais e fornecemos raciocínio analítico para o comportamento dessa média. Além disso, fornecemos um método comprovado para calcular o emaranhamento em cadeias de spin que têm interação não uniforme com campos magnéticos externos nos limites. Os modelos mencionados são conhecidos por serem difíceis de resolver e estudar. Nós fornecemos (e provamos) uma fórmula para reduzir drasticamente a dificuldade de calcular a matriz de densidade reduzida e o emaranhamento de contorno em tais sistemas. Este trabalho fornece um método concreto e fácil para estudar ainda mais o emaranhamento dos modos de borda de Majorana e outros sistemas relacionados na física quântica de muitos corpos.

Palavras-chaves: Cadeias de spins. Férmions quadráticos. Correlação quântica. Operador densidade. Matriz densidade. Entrelaçamento quântico. Emaranhamento quântico.

Abstract

The XY spin chains and related quadratic fermion models have been studied vastly during the last 70 years ago. In this thesis, the solution and the connection between the solvable XY spin model and quadratic fermions, obtain by the Jordan-Wigner fermionization, are reviewed in detail. The family of XY spin chain, such as the quantum Ising chain and XX spin chain, have been a huge part of quantum manybody physics and quantum information. After presenting the solution to the diagonalization of the XY spin chain and the fermionic model, other methods of the formulation of eigenstates of these systems are presented. I also discuss the correlation function contents of these models, and it is not limited to ground state only. Different formulations of density matrix operator are also presented in the most comprehensive way. All the mentioned quantities are then used to study the bipartite entanglement of these modes. The second part of the thesis (published articles part) contains the applications of the methods provided in the earlier parts to particularly study the entanglement in this family of models. For instance, we have studied the universal average entanglement entropy over all eigenstates of the general fermionic models in $1D$ and provided analytical reasoning for the behavior of this averaging. It was proved that these models, independent of the gap, have infinite excited states that can be described by conformal field theory. In addition, we have provided a proven method to calculate the entanglement in spin chains that have non-uniform interaction with external magnetic fields at the boundaries. The models mentioned are known to be challenging to solve and study. We provide (and proof) a formula to reduces the difficulty of calculating the reduced density matrix and boundary entanglement in such systems drastically. This work dispenses a concrete and easy method to further study entanglement of Majorana edge modes and other related systems in manybody quantum physics.

Key-words: Quantum spin chains. Quadratic fermions. Correlation functions. Density matrix operator. Entanglement.

Lista de ilustrações

Lista de tabelas

Sumário

— 1 —

Introduction

Quantum mechanics' correlations have no classical analogue and are one of the most fascinating discoveries of the 20^{th} century. The existence of such correlations, called entanglement, was revealed by the famous Einstein-Podolsky-Rosen (EPR) Gedanken experiment in the 1930s [1], which could not be explained by any classical theory. Even it was considered by Einstein as a "*spooky action at a distance*" at that time. Nowadays, the notion of entanglement has transformed into a well-established concept. The kick-off for this development was the inequalities formulated by Bell in 1964 [2]. Violation of a Bell inequality implies the existence of quantum mechanical correlations that leads to quantum entanglement. Over twenty years later, the first convincing experiment proving the violation of a Bell inequality was performed (by Aspect) [3, 4]. Aspect's experiments gave rise to the advent of quantum information theory in the early 1990s, where the quantum correlations and quantum entanglement played the role of resource for many technological applications. Since that time, quantum information science has developed into a popular research area, ranging from foundational questions of the interpretation of quantum mechanics to the search for the technological application of entanglement [5].

With the beginning of the 21st century intriguing experiments using ultracold quantum gases (see [6] for a review) were an immense success for this field of science, and attracted the attention of the quantum information and condensed matter community. The groundbreaking realization of a Bose-Einstein condensate in a system of Rubidium atoms revolutionized condensed matter physics. The present experiments with bosonic and fermionic atoms offer an exciting possibility to verify concepts predicted by the theory of condensed matter physics and allow to discover and explore new and exotic quantum phases. Furthermore, realization of cold atoms led to the immense success of quantum computations. Certain computational tasks, such as simulating quantum mechanical systems, can be done exponentially faster using an ultracold atom setup or quantum computer based on qubits than by a classical computer [7]. However, the experimental realization of a large-scale quantum computer capable of accomplishing those tasks is still an unsolved task.

The study of entanglement in quantum many-body systems has become one of the major efforts in the physics community, due to its potential for describing quantum phases of matter and topological order [8, 9, 10, 11]. Characterizing entanglement in many-body systems is still an open field of research (see [12] for a review). The situation gets more complicated when the particles or size of the system under consideration grows. Calculation of entanglement entropy, even bipartite entanglement for pure states grows with the size of the system. In particular, knowing the entanglement relies on finding the eigenvalues of a matrix that grows exponentially with the size of the system, let alone the fact that finding eigenvalues is a complicated computational process. The application of tools and techniques from various fields of physics, and mathematics into the condensed matter physics resulted

in interesting insights in calculating the entanglement for manybody systems, specially fermionic systems. Fermions, which are the basic building blocks of matter, are central to many of the most fascinating effects in condensed matter physics, like superconductivity, superfluidity, or the quantum Hall effect. In this regard, free fermionic systems are especially interesting, as there have been theoretically proven relations which allow one to write the density matrix and calculate the entanglement with less computational efforts [13, 14, 15]. Consequently, the investigation and study of quantum aspects in many fermionic systems are the main focus of this Thesis.

The important components of this thesis are organized as follows. The first part, the prerequisites part, is devoted to educate the reader on the models and methods. It can be thought of as a self-sufficient review of the spin and fermionic chain materials in which relations are explained well, equations are opened up and derived in easy steps, and examples have been given. In chapter 2, the XY spin model and related spin models are presented in detail, then the connection of these spin chains to fermionic models is cleared up. Then I discuss the quadratic fermions and their solution in extension. I stick to the most general case possible, and after explaining the diagonalization process, I go into the means to represent the eigenstates of the system and possible constraints. End of the first chapter spin chains are revisited, and it focuses on obtaining the spectrum of the spin system from that of the fermion system. Chapter 3 is devoted to the study of the correlation function for quadratic fermions and related spin chains. Chapter 4 introduces different formulations of density matrix and reduced density matrix, which uses the results of previous chapters. The final chapter of part I, briefly talks about the quantum entanglement in manybody systems, and some useful relations are presented. In part II of this thesis, published papers are located. In chapter 6 (Ref. [16]) we investigated the averaging of the subsystem entanglement entropy over all excited states of general free fermion models. In particular, firm reasoning is proposed for the behavior of mentioned averaging, which is valid for the most general case of free fermion and related spin chains. In chapter D (Ref. [17]), we took the advantage of the methods and formulations of free fermions to prove a new ansatz for reduced density matrix which reduces the difficulty of studying the entanglement in spin systems with diverging boundary magnetic field in 1D. The boundary entanglement contains more information than conventional belief.

Parte I

Prerequisites

— 2 —

Integrable spin chains and free fermions

2.1 Solvable Spin Chains

Historically, the realization of spin interactions goes back to the works in the early stages of quantum mechanics such as works by Heisenberg and Dirac's works [18, 19]. These interactions were found to be arising instinctively between electrons of nearby atoms, and it could explain the ferromagnetism concept. In 1931, Hans Bethe published the first exact solution of a many-body quantum system [20], known as the spin-$\frac{1}{2}$ Heisenberg model. Bethe's work inspired many scientists in mathematics and theoretical physics and started a new branch of physics, the theory of exactly solvable models. For instance, in 1979, Fadeev, Sklyanin, and Takhtadzhyan formulated the algebraic version of the Bethe ansatz [21, 22], which is a remarkable method. Solvability in many-particle quantum systems is very important. On the one hand, the exactly solvable models can have analytical and/or exact numerical results that can be used to extract information from the system; on the other hand, these solvable models open the door for a better understanding of quantum many particle systems.

Although the Bethe ansatz was revolutionary in the realm of quantum mechanics, the solutions coming from (algebraic) Bethe ansatz are quite involved and complicated. In the rest of the work, I will not consider models solvable in the sense of Bethe ansatz. The interesting physical quantities in this thesis, namely the correlation matrices, formulation of the density matrix, and entanglement properties, do not generally find a useful solution in the framework of (algebraic) Bethe ansatz. In fact, I will use a different approach to the problem of interacting spin-$\frac{1}{2}$'s, coming from the similarity between spin-$\frac{1}{2}$ and fermion operators [23]. This thesis is intended as a guide to those specific models that can be mapped into non-interacting fermion systems. The rest of this chapter is devoted to first, the study of the XY model, second, study of quadratic fermion models.

2.2 XY model

The quantum XY spin chain and its extensions have been studied for a very long time and from various perspectives. they are interesting for couple of reasons. First of all, it is possible to obtain an exact solution (for spin one-half) in terms of non-interacting fermions [24]. Also, it can be used in examining various techniques that are applied to a wide range of non-integrable systems [25]. Another motivation could be to use the model to describe the experimental data of quasi-one-dimensional systems [26]. In recent years the XY chain has been extensively examined in the context of quantum information theory and quantum entanglement entropy [27, 28, 29, 30, 31, 32].

The XY model is a quantum spin-$\frac{1}{2}$ chain formulated by the Hamiltonian

$$H_{XY} = -J \sum_{n,m} \left(\frac{1+\gamma}{1} S_n^x S_m^x + \frac{1-\gamma}{1} S_n^y S_m^y \right) - h \sum_n S_n^z \tag{2.1}$$

where $S_l^\alpha = \frac{1}{2}\sigma_l^\alpha$ $(\alpha = x, y, z)$ and σ^αs are the Pauli matrices. J is the coupling constant, which specifies the interaction of each spin with neighboring ones, h is known as the transverse magnetic field, and γ is the coupling constant, altering the weight of $x - y$ component of the interaction between neighboring spins. Although the form of Hamiltonian above is written for a general D-dimension system with possible long range interactions, throughout this thesis we only consider spin models in one spatial dimension (1D) and only the next nearest interactions. For 1-dimension, the Hamiltonian above can be written as

$$H_{XY} = -J\sum_{l=1}^{L}\left(\frac{1+\gamma}{4}\sigma_l^x\sigma_{l+1}^x + \frac{1-\gamma}{4}\sigma_l^y\sigma_{l+1}^y\right) - \frac{h}{2}\sum_{l=1}^{L}\sigma_l^z, \tag{2.2}$$

where spin operators are swapped for the Pauli matrix operators σ. The boundary condition in the 1D system can be open, called an open chain, or periodic which means spins are located on a circle. Mathematically, the boundary condition can be manifested in the spin σ_{L+1}^α. Either it is replaced by σ_1^α for periodic boundary condition (PBC) or non-existence (zero), for the open (OBC) system.

In the context of the energy spectrum, the sign of the coupling J in the XY model is not important. Meaning that the energy spectrum of the ferromagnetic phase ($J < 0$) is the same as the spectrum of anti-ferromagnetic ($J > 0$). However, the sign of J can not be neglected for the eigenstates of ferromagnetic ($|\psi\rangle$) and anti-ferromagnetic ($|\psi'\rangle$) case. The reasoning is explained in the following subsection. In short, there exist transformations that change the sign of coupling constants in the system. Because of the existence of these particular transformations, without loss of generality, J can be scaled to $+1$ (or -1) and one could only study the properties of this model for the $h \geq 0$ region (or $h \leq 0$). For $\gamma = 0$, the XY model is called the XX model (see section 2.2.4 for more details). When $\gamma = +1$, the XY model is called the Ising model and a more detailed explanation of its properties can be found in section 2.2.3. The phase diagram for the XY ground state is shown in figure 1. A detailed reference regarding the origin of all phases (especially the oscillatory phase) is [33, 34].

2.2.1 Symmetries and general transformations

The XY model shows some global invariance. In particular, the global symmetries depend on the value of γ. For start, if $\gamma = 0$, then H_{XY} is invariant under a global $U(1)$ transformation

$$\begin{pmatrix}\sigma'^x\\ \sigma'^y\\ \sigma'^z\end{pmatrix} = \begin{pmatrix}\cos\theta & -\sin\theta & 0\\ \sin\theta & \cos\theta & 0\\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix}\sigma^x\\ \sigma^y\\ \sigma^z\end{pmatrix} \tag{2.3}$$

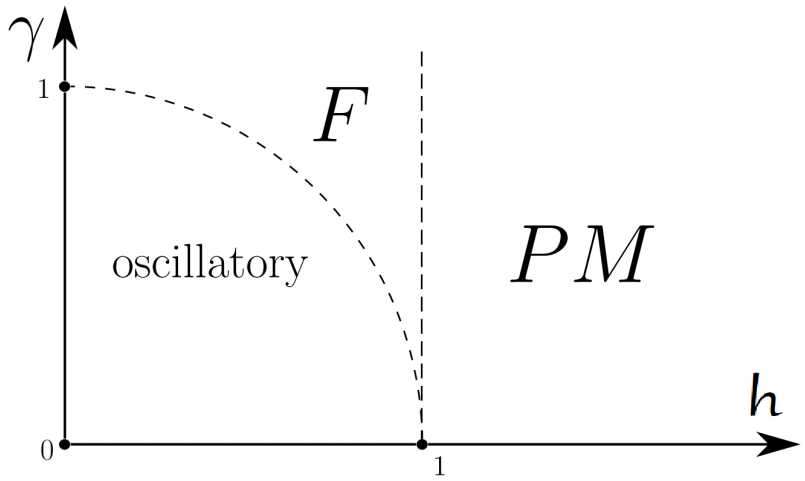


Figure 1 – The phase diagram of the ferromagnetic XY chain. One can distinguish three phases, i.e. a ferromagnetic phase (F), which divides to oscillatory and non oscillatory regions, and a paramagnetic phase (PM). Parameters h and γ are the magnetic field strength and anisotropy parameter respectively. Figure from [34].

where θ is an arbitrary real number. If $\gamma \neq 0$, one only has a global $\mathbb{Z}_2$ invariance

$$\begin{pmatrix} \sigma'^x \\ \sigma'^y \\ \sigma'^z \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \sigma^x \\ \sigma^y \\ \sigma^z \end{pmatrix}. \tag{2.4}$$

This symmetry can be produced by

$$P = \prod_{j=1}^{L} \sigma_j^z \tag{2.5}$$

which is also known as the *Parity* operator and it is shown that $[H_{XY}, P] = 0$. The $\mathbb{Z}_2$ invariance is obvious for the $\gamma \neq 0$. Since $\sigma_i'^z \to \sigma_i^z$ and $\sigma_i'^\alpha \sigma_{i+1}'^\alpha$ does not change $(\alpha = x, y)$. The $\mathbb{Z}_2$ symmetry is present in almost all physical systems. An interesting study of non-parity cases in a spin system can be found in chapter 7. For $U(1)$ symmetry in the case of $\gamma = 0$ we have:

$$\begin{aligned} H'_{XY} = &-\frac{J}{4}\sum_{l=1}^{L}\left(\sigma_l'^x\sigma_{l+1}'^x + \sigma_l'^y\sigma_{l+1}'^y\right) = -\frac{J}{4}\sum_{l=1}^{L}\Big([\cos\theta\sigma_l^x - \sin\theta\sigma_l^y] \\ &[\cos\theta\sigma_{l+1}^x - \sin\theta\sigma_{l+1}^y] + [\sin\theta\sigma_l^x + \cos\theta\sigma_l^y][\sin\theta\sigma_{l+1}^x + \cos\theta\sigma_{l+1}^y]\Big) \\ = &-\frac{J}{4}\sum_{l=1}^{L}\left([\cos^2\theta + \sin^2\theta]\sigma_l^x\sigma_{l+1}^x + [\cos^2\theta + \sin^2\theta]\sigma_l^y\sigma_{l+1}^y\right) = H_{XY} \end{aligned}$$

It should be noted that here we omitted the last term in H_{XY} since it only contains the σ_z, and $U(1)$ symmetry has no effect on the z-component of spin.

As it was pointed out earlier, in contrast to the well-known Heisenberg spin model, where the sign of the coupling constant J distinguishes the ferromagnetic model from the

anti-ferromagnetic one, the sign of J in the XY model is unimportant. It can be shown by the existence of the transformation

$$P_J \equiv \prod_{l=odd\,(even)}^{L} \sigma_l^z \tag{2.6}$$

which changes the sign of the coupling constant J. Clearly, transformation P_J has no action on the last term of Hamiltonian equation (2.2). Using $\sigma^a\sigma^b = \delta_{a,b}\mathbb{1} + i\varepsilon_{abc}\sigma^c$, we will examine the effect of this similarity transformation on other terms of Hamiltonian separately:

$$P_J\Big(\sum_{l=1}^{L}\sigma_l^x\sigma_{l+1}^x\Big)\tilde{P}_J = \sum_{l=1}^{L}\prod_{n=1}^{\lfloor L/2\rfloor}\sigma_{2n-1}^z\sigma_l^x\sigma_{l+1}^x\sigma_{2n-1}^z = \sum_{l=1}^{L}-\sigma_l^x\sigma_{l+1}^x$$
$$P_J\Big(\sum_{l=1}^{L}\sigma_l^y\sigma_{l+1}^y\Big)\tilde{P}_J = \sum_{l=1}^{L}\prod_{n=1}^{\lfloor L/2\rfloor}\sigma_{2n-1}^z\sigma_l^y\sigma_{l+1}^y\sigma_{2n-1}^z = \sum_{l=1}^{L}-\sigma_l^y\sigma_{l+1}^y$$

Therefore, we can show that

$$P_J H_{\mathrm{XY}}(J,h)P_J^\dagger = H_{\mathrm{XY}}(-J,h). \tag{2.7}$$

Above relation and the fact that P_J is a normalized similarity transformation ($P_JP_J^\dagger = \mathbb{1}$) I can argue that:

$$H_{\mathrm{XY}}(J,\gamma,h)\,|\psi\rangle = E_\psi\,|\psi\rangle$$
$$P_JP_J^\dagger H_{\mathrm{XY}}(J,\gamma,h)P_JP_J^\dagger\,|\psi\rangle = E_\psi P_JP_J^\dagger\,|\psi\rangle$$
$$P_J H_{\mathrm{XY}}(-J,\gamma,h)P_J^\dagger\,|\psi\rangle = P_J E_\psi P_J^\dagger\,|\psi\rangle$$
$$H_{\mathrm{XY}}(-J,\gamma,h)\,|\psi'\rangle = E_\psi\,|\psi'\rangle$$

where $|\psi'\rangle = P_J^\dagger\,|\psi\rangle$ and Hamiltonian $H_{\mathrm{XY}}(-J,\gamma,h)$ corresponds to anti-ferromagnetic model. We see that the ferromagnet system ($J>0$) and anti-ferromagnet one ($J<0$), both have the same energy spectrum E_ψ.

Similar to the P_J case, the transformation

$$P_h \equiv \prod_{l=1}^{L}\sigma_l^x \tag{2.8}$$

changes the sign of the magnetic field coupling h. To show this, we start with the fact that transformation P_h has no action on the first term of Hamiltonian (2.2). We will examine the effect of this similarity transformation on other terms of Hamiltonian separately, likewise.

$$P_h\Big(\sum_{l=1}^{L}\sigma_l^z\Big)P_h^\dagger = \sum_{l=1}^{L}\prod_{n=1}^{L}\sigma_n^x\sigma_l^z\sigma_n^x = \sum_{l=1}^{L}-i\sigma_l^y\sigma_l^x = \sum_{l=1}^{L}(-i)^2\sigma_l^z = \sum_{l=1}^{L}-\sigma_l^z$$

The action of P_h on the y-spin interactions does not change anything. Therefore, we have:

$$P_h H_{\mathrm{XY}}(J,h)P_h^\dagger = H_{\mathrm{XY}}(J,-h) \tag{2.9}$$

Like the P_J case, the sign of h does not affect the structure of the energy spectrum in the XY model.

Following the same procedure, it is possible to write a transformation such as P_γ which changes the sign of the coupling γ:

$$P_\gamma \equiv \prod_{l=1}^{L} \frac{1}{\sqrt{2}}(1 + i\sigma_l^z). \tag{2.10}$$

Then

$$\begin{aligned} P_\gamma \sum_{l=1}^{L} \sigma_l^x \sigma_{l+1}^x P_\gamma^\dagger =& \frac{1}{4}\sum_l (1 + i\sigma_l^z)\sigma_l^x(1 - i\sigma_l^z)(1 + i\sigma_{l+1}^z)\sigma_{l+1}^x(1 - i\sigma_{l+1}^z) \\ =& \frac{1}{4}\sum_l (\sigma_l^x + i\sigma_l^z\sigma_l^x - i\sigma_l^x\sigma_l^z + \sigma_l^z\sigma_l^x\sigma_l^z)(\sigma_{l+1}^x + i\sigma_{l+1}^z\sigma_{l+1}^x \\ & - i\sigma_{l+1}^x\sigma_{l+1}^z + \sigma_{l+1}^z\sigma_{l+1}^x\sigma_{l+1}^z) = \frac{1}{4}\sum_l (\sigma_l^x + (i)^2\sigma_l^y - i(-i)\sigma_l^y - \sigma_l^x) \\ & \times (\sigma_{l+1}^x + (i)^2\sigma_{l+1}^y - i(-i)\sigma_{l+1}^y - \sigma_{l+1}^x) = \sum_l \sigma_l^y\sigma_{l+1}^y, \end{aligned}$$

and similarly, for the y-spin interaction we have

$$P_\gamma \sum_{l=1}^{L} \sigma_l^y \sigma_{l+1}^y P_\gamma^\dagger = \sum_l \sigma_l^x\sigma_{l+1}^x.$$

As you can see, this transformation changes $\sigma_l^x\sigma_{l+1}^x$ to $\sigma_l^y\sigma_{l+1}^y$ and vice-versa which is the same as changing $\gamma \to -\gamma$ in Hamiltonian (2.2). As one can notice, the action of P_γ on the last term of the equation (2.2) does not change this term.

All the transformations introduced earlier (P_J, P_h and P_γ) are *Similarity* transformations, $A' = P_\alpha A P_\alpha^{-1}$. They all satisfy the conjugate condition

$$P_\alpha P_\alpha^\dagger = \mathbb{1} \tag{2.11}$$

More accurately, They can be called *Canonical transformation*, meaning they do not change the algebra. However, P_J and P_h, defined earlier, are Involutory matrices (Projection), $P_J P_J = P_h P_h = \mathbb{1}$ but P_γ is Unitary ($P_\gamma P_\gamma^\dagger = \mathbb{1}$). Each of these transformations was introduced to change a particular coupling of the system, although for some of the required changes transformation is not unique. For instance, $P_h' \equiv \prod_{l=1}^{L} \sigma_l^y$ also does change the sign of magnetic field's coupling constant.

Here we intend to write these transformations and probably others that we have not encountered yet, in a more general form. This way, we can discuss more general transformation and symmetries of interest. To start let's write the most inclusive form of the Euler formula

$$e^{i\alpha(\hat{n}\cdot\vec{\sigma})} = \mathbb{1}\cos\alpha + i(\hat{n}\cdot\vec{\sigma})\sin\alpha \tag{2.12}$$

which $|\hat{n}| = 1$. Having this, we can write the former transformations in a generic form. Before going any further we have to rewrite the previous transformations. For instance

$$P_J = \prod_{l=1}^{\lfloor \frac{L}{2} \rfloor} i\sigma_l^z \quad \text{and} \quad P_h = \prod_{l=1}^{L} i\sigma_l^x = \prod_{l=1}^{L} i\sigma_l^y \tag{2.13}$$

this new P_J and P_h are unitary and still deliver the same result as before. Now we can write

$$P_h = \prod_{l=1}^{L} i\sigma_l^x = \prod_{l=1}^{L} e^{i\frac{\pi}{2}(\hat{n}_1 \cdot \vec{\sigma}_l)}, \qquad \begin{matrix} \hat{n}_1 = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \\ \vec{\sigma}_l = \begin{pmatrix} \sigma_l^x & \sigma_l^y & \sigma_l^z \end{pmatrix} \end{matrix}$$

or consequently

$$P_\gamma = \prod_{l=1}^{L} \frac{1 + i\sigma_l^z}{\sqrt{2}} = \prod_{l=1}^{L} e^{i\frac{\pi}{4}(\hat{n}_\gamma \cdot \vec{\sigma}_l)}, \qquad \hat{n}_\gamma = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix}.$$

Another interesting outcome of such a notation could be the case $\hat{\mathcal{N}}' = \prod_{l=1}^{L} i\sigma_l^z$. We have named this transformation as $\mathcal{N}'$. The reason is not going to be discussed in this part but in the section 2.4, this operator is going to play an important role in solving the XY-Hamiltonian.

$$\hat{\mathcal{N}}' = \prod_{l=1}^{L} i\sigma_l^z = \prod_{l=1}^{L} e^{i\frac{\pi}{2}(\sigma_l^z)} = e^{i\frac{\pi}{2}(\sigma_1^z)} e^{i\frac{\pi}{2}(\sigma_2^z)} \cdots e^{i\frac{\pi}{2}(\sigma_L^z)} = e^{i\frac{\pi}{2}S^z} \tag{2.14}$$

Where S^z is the total spin in the z direction and $\mathcal{N}$ is the $\mathbb{Z}_2$ transformation generator (later we are going to see that $[\mathcal{N}', H_{XY}] = 0$).

With equation (2.12) it is helpful to investigate the action of a general transformation $P_\alpha = \prod_j e^{i\alpha(\hat{n}\cdot\vec{\sigma}_j)}$ on H_{XY}. It is also straightforward to look at the adjoint action of P_α on the Pauli vector, namely rotation effectively by double the angle α

$$e^{i\alpha(\hat{n}\cdot\vec{\sigma}_l)} \vec{\sigma}_l e^{-i\alpha(\hat{n}\cdot\vec{\sigma}_l)} = \vec{\sigma}_l \cos(2\alpha) + \hat{n} \times \vec{\sigma}_l \sin(2\alpha) + \hat{n}(\hat{n} \cdot \vec{\sigma}_l)(1 - \cos 2\alpha) \tag{2.15}$$

then we can write

$$\begin{aligned} P_\alpha H_{XY} P_\alpha^\dagger = &- J \sum_{l=1}^{L} \Big(\frac{1+\gamma}{4} e^{i\alpha(\hat{n}\cdot\vec{\sigma}_l)} \sigma_l^x e^{-i\alpha(\hat{n}\cdot\vec{\sigma}_l)} e^{i\alpha(\hat{n}\cdot\vec{\sigma}_{l+1})} \sigma_{l+1}^x e^{-i\alpha(\hat{n}\cdot\vec{\sigma}_{l+1})} \\ &+ \frac{1-\gamma}{4} e^{i\alpha(\hat{n}\cdot\vec{\sigma}_l)} \sigma_l^y e^{-i\alpha(\hat{n}\cdot\vec{\sigma}_l)} e^{i\alpha(\hat{n}\cdot\vec{\sigma}_{l+1})} \sigma_{l+1}^y e^{-i\alpha(\hat{n}\cdot\vec{\sigma}_{l+1})} \Big) - \frac{h}{2} \sum_{l=1}^{L} e^{i\alpha(\hat{n}\cdot\vec{\sigma}_l)} \sigma_l^z e^{-i\alpha(\hat{n}\cdot\vec{\sigma}_l)} \end{aligned} \tag{2.16}$$

Since we are interested to see explicitly what happens to our Hamiltonian after this transformation, we will attempt to simplify the above relation. Although it is not possible to write the former in a compact equation, we can write in symbolic form. For instance:

$$P_\alpha H_{XY} P_\alpha^\dagger = - J \sum_{l=1}^{L} \overrightarrow{\sigma}_l^T \mathcal{A} \overrightarrow{\sigma}_{l+1} - \frac{h}{2} \sum_{l}^{L} \mathcal{B} \overrightarrow{\sigma}_l. \tag{2.17}$$

This is a matrix product with $\overrightarrow{\sigma}_i^T = \begin{pmatrix} \sigma_i^x & \sigma_i^y & \sigma_i^z \end{pmatrix}$. For $\mathcal{A}$ and $\mathcal{B}$ we have:

$$\mathcal{A} = \begin{pmatrix} A_{XX} & A_{XY} & A_{XZ} \\ A_{YX} & A_{YY} & A_{YZ} \\ A_{ZX} & A_{ZY} & A_{ZZ} \end{pmatrix} \quad \mathcal{B} = \begin{pmatrix} B_X & B_Y & B_Z \end{pmatrix}$$

Before going through the explicit form of these elements, we should elaborate a few words on this. Technically, our new Hamiltonian contains all possible interactions. For instance, A_{ZZ} is the interaction coupling between σ_l^z and σ_{l+1}^z. Conversely, A_{XY} is the interaction intensity between σ_l^x and σ_{l+1}^y (same argument is valid for $\mathcal{B}$). Not all the possible interactions are interesting or even physical. By tunning parameters like α and $\hat{n}$ one can turn some of interactions on or off as needed. The A's and B's explicit expressions are given in Appendix B. We can check this result with known cases, for example $\alpha = 0$ and $\hat{n} = (0, 0, 0)$.

$$\mathcal{A} = \begin{pmatrix} \frac{1+\gamma}{4} & 0 & 0 \\ 0 & \frac{1-\gamma}{4} & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \mathcal{B} = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix}$$

which is the original Hamiltonian. Also, For P_h (left, $\alpha = \frac{\pi}{2}$ and $\hat{n} = \hat{x}$) and P_γ (right, $\alpha = \frac{\pi}{4}$ and $\hat{n} = \hat{z}$) we have:

$$\mathcal{A}_h = \begin{pmatrix} \frac{1+\gamma}{4} & 0 & 0 \\ 0 & \frac{1-\gamma}{4} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \mathcal{A}_\gamma = \begin{pmatrix} \frac{1-\gamma}{4} & 0 & 0 \\ 0 & \frac{1+\gamma}{4} & 0 \\ 0 & 0 & 0 \end{pmatrix},$$
$$\mathcal{B}_h = \begin{pmatrix} 0 & 0 & -1 \end{pmatrix}, \qquad \mathcal{B}_\gamma = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix}.$$

Special cases:

- For arbitrary $\hat{n}$ but $\alpha = k\pi$, Hamiltonian does not change.
- For $\hat{n} = n_z$ but $\alpha = k\frac{\pi}{2}$, Hamiltonian does not change.
- For $\hat{n} = 0$ but arbitrary α, Hamiltonian does not change.

2.2.2 Computation and Examples

In this section, first, we are going to construct the Hamiltonian of the XY-model and then look at some easy cases ($L = 2, 3$). For L spins arranged in one dimension, we have a 2^L dimensional configuration space. The natural basis set for describing a set of L coupled spins is the tensor-product basis. In this basis, the spin operators $\sigma_j^{x,y,z}$ acting only on spin j are defined as having a trivial action on all other spins except the site j, for example

$$S_j^\alpha \to \underbrace{\mathbb{1} \otimes \cdots \otimes \mathbb{1}}_{j-1} \otimes \tfrac{1}{2}\sigma_j^\alpha \otimes \underbrace{\mathbb{1} \otimes \cdots \otimes \mathbb{1}}_{L-j}, \tag{2.18}$$

or like wise,

$$S_i^\beta S_j^\alpha \to \underbrace{\mathbb{1}\otimes\cdots\otimes\mathbb{1}}_{i-1}\otimes\tfrac{1}{2}\sigma_i^\beta\otimes\underbrace{\mathbb{1}\otimes\cdots\otimes\mathbb{1}}_{i-j-1}\otimes\tfrac{1}{2}\sigma_j^\alpha\otimes\underbrace{\mathbb{1}\otimes\cdots\otimes\mathbb{1}}_{L-i-j}, \tag{2.19}$$

where $\alpha,\beta\in\{x,y,z\}$, depending on the model.

Unless otherwise stated, we prefer to work in the basis of z-spin. At some point, if we wish to work in another basis such as eigenstates of x-spin, we can relabel the indices according to $S_{x'}=S_z$, $S_{y'}=-S_y$ and $S_{z'}=S_x$. Thus the eigenstates of $\sigma_{x'}$ are just the eigenstates of σ_z. In the following, for demonstration and better understanding purposes, we consider the example of a small spin chain. To see some examples of the computational parts, see appendix B.

2.2.3 Ising model

The quantum Ising model is famous in the family of XY spin chains. It is obtained by putting $\gamma=1$ in the Hamiltonian (2.2):

$$H_{Ising}=-\frac{J}{2}\sum_{l=1}^{L}\sigma_l^x\sigma_{l+1}^x-\frac{h}{2}\sum_{l=1}^{L}\sigma_l^z. \tag{2.20}$$

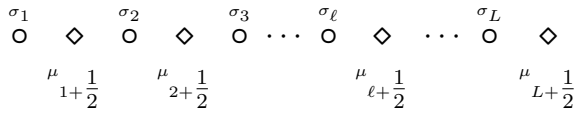
This model is widely used to study quantum critical behaviors [35] and a play model for CFT predictions [36, 37]. The ground state of the quantum Ising models shows a second-order quantum phase transition when the magnetic field is increased from zero to the critical value of $h_c=J$, in the thermodynamic limit ($L\to\infty$) [38, 39]. The existence of this critical point can be explained as follow. In zero (or very small) magnetic fields ($|h|\ll 1$), there are two degenerate ground states for the ferromagnetic ordered phase, all spins are aligned parallel to each other in the x-direction (either $|{\to}{\to}\cdots{\to}\rangle$ or $|{\leftarrow}{\leftarrow}\cdots{\leftarrow}\rangle$). By increasing the magnetic field ($h\gg J$), the ground state would be non-degenerate, and the spins are aligned in the z direction (direction of magnetic field). This argument suggests that one can not go from one ground state to the other smoothly by changing the magnetic field, which corresponds to a second-order quantum phase transition [38, 39].

The existence of the quantum critical point can be also proved via the duality in this model. Duality is the equivalence of two Hamiltonians with different parameters. In particular, we are talking about the Kramers-Wannier duality which is originally the equivalence of low temperature to high temperature in the Ising model [40]. A comprehensive exposition on duality can be found in [41]. In the case of quantum Ising this duality means there is a critical point going from low magnetic fields to high magnetic fields [42, 43]. To show this, we first add a term to the Ising Hamiltonian (2.20):

$$H_{Ising}=-\frac{J}{2}\sum_{l=1}^{L}\sigma_l^x\sigma_{l+1}^x-\frac{h}{2}\sum_{l=1}^{L}\sigma_l^z-\frac{J}{2}\sigma_1^x\prod_{j=1}^{L}\sigma_j^z\sigma_L^x. \tag{2.21}$$

The last term was added to make it possible to go through Kramers-Wannier duality and take care of some terms which are going to pop up. Also, it should be emphasized that boundary condition is assumed to be periodic. For the case of OBC, the extra terms which should be added are either $-\frac{J}{2}\sigma_L^x$ or $+\frac{h}{2}\sigma_L^z$.

To get to the dual version of the system, on our (1D) lattice (PBC or OBC), we make a dual lattice, by putting a new particle $\mu_{_{i+1/2}}$ in between each two spins σ_i and σ_{i+1}.



The new operator μ associated with the new particles has the definition:

$$\mu_{j+1/2}^z = \sigma_j^x \sigma_{j+1}^x, \qquad \mu_{j+1/2}^x = \prod_{k\leq j} \sigma_k^z. \tag{2.22}$$

With above definitions, we can verify that

$$[\mu_i^x, \mu_j^z] \propto \delta_{ij}, \qquad \{\mu_i^x, \mu_i^z\} = 0, \quad \text{and} \quad \mu_j^{z2} = \mu_i^{x2} = 1.$$

In fact, μ^α operators have the same algebra as the Pauli matrices. To have a complete algebra, one can get the μ^y by

$$i\mu_i^y = [\mu_i^z, \mu_i^x]. \tag{2.23}$$

At this point, we are not interested in the μ^y at all and we would not proceed further in demonstrating the $SU(2)$ algebra for μ^α operators.

By writing the σ operators in terms of μ operators and substituting in the Hamiltonian (2.21), we get (after some simplifications)

$$\tilde{H}_{Ising} = -\frac{J}{2}\sum_{l=1}^{L} \mu_{l+1/2}^z - \frac{h}{2}\sum_{l=1}^{L} \mu_{l-1/2}^x \mu_{l+1/2}^x. \tag{2.24}$$

As a consequence, $H(J,h;\sigma) = \tilde{H}(h,J;\mu)$. By putting $\lambda = \frac{h}{J}$, then:

$$H_{Ising}(\lambda;\sigma) = \lambda \tilde{H}_{Ising}(\frac{1}{\lambda};\mu). \tag{2.25}$$

Therefore, Kramer duality maps the high magnetic field to the weak magnetic field, which is also called the *Strong-Weak* duality. The energy spectrum of dual Hamiltonians should be related analogously as $E_j(\lambda) = \lambda E_j(\frac{1}{\lambda})$. It means that the distance between two energy values $\Delta(\lambda) = E_j - E_{j+1}$ should have equal behavior. Particularly for the ground state and the first excited state have:

$$\Delta(\lambda) = \lambda\, \Delta(\frac{1}{\lambda}). \tag{2.26}$$

In the most general case, the function $\Delta(\lambda)$ should have the form below

$$\Delta(\lambda)|\lambda^a - \frac{1}{\lambda^b}|^c; \qquad \begin{cases} \frac{1}{c} + b = a \\ \frac{1}{c} - a = -b \end{cases}. \tag{2.27}$$

The form above has two solutions for $\Delta(\lambda) = 0$, given by $\lambda = 0, 1$. Roots of $\Delta(\lambda)$ establish that there should be a value for parameter λ where the gap between the ground state and the first excited one goes to zero. This gap closing shows the existence of a critical point, namely $J = h$. Finally, this duality is valid also for non-uniform or non-local coupling constant, $\{J, h\} \to \{J_l, h_l\}$.

2.2.4 XX model

The XX model is the anisotropic regime of equation (2.2) with $\gamma = 0$:

$$H_{XX} = -\frac{J}{4}\sum_{l=1}^{L}\left(\sigma_l^x\sigma_{l+1}^x + \sigma_l^y\sigma_{l+1}^y\right) - \frac{h}{2}\sum_{l=1}^{L}\sigma_l^z. \tag{2.28}$$

This model has application in various parts of quantum many-body and condensed matter physics and quantum information [44, 45]. As an example, it is related to the hard-core limit of the one-dimensional Bose-Hubbard model [39]. The XX Hamiltonian (2.28) is mapped into the Bose-Hubbard Hamiltonian:

$$H_{B.H.} = -\frac{J}{2}\sum_{<i,j>}\left(b_i^\dagger b_j + b_i b_j^\dagger\right) + \frac{U}{2}\sum_i n_i(1-n_i) + \mu\sum_i n_i \qquad n_i = b_i^\dagger b_i, \tag{2.29}$$

where b_i is a spinless boson. This bosonic model was realized experimentally by Greiner et al [46] in 2002 and provided the simplest realization of a quantum phase transition. For more information see [35], also [39] page 27.

On the characteristics of this model, the total spin in the z-direction, $S^z = \frac{1}{2}\sum_{l=1}^{L}\sigma_l^z$, commutes with the XX Hamiltonian,

$$[S^z, H_{XX}] = 0.$$

It means that the eigenstates of XX models sit in the different sectors based on the value of S^z. independent of the magnetic field h, Hamiltonian (2.28) is block diagonal in the S_z basis. This model is critical for any value of $|h| \leq J$ with the central charge of $c = 1$ [39]. However, for $|h| \gg J$, all spins are aligned in the z-direction in the ground state and it is not critical in this regime.

Together with the connection to different many-body models, the XX model is favorable because of its mathematical simplicity but still non-triviality. With no doubt, many of the existing manybody predictions, such as subsystem entanglement entropies and full counting statistics, have been obtained and verified considering XX spin chain [39, 47, 16, 48]. Another point is the diagonalization of this model (after the fermionization) for periodic and open boundary conditions, which allows further simplifications for the XX model (see sections 2.4.1 and 2.4.2). In conclusion, specific mathematical features of spin models such as the XX model and Ising model make the XY model an archetype of integrable spin models. I am going to describe the fermionic mapping of the XY model in the following subsection.

2.2.5 Fermionic mapping

In this part, the fermionizatoin of the XY model will be discussed. The XY model can be solved exactly by mapping the Hilbert space of L spins-$\frac{1}{2}$ to the Fock space of L spinless fermions [24, 39, 49]. This fermionization is assigning a new fermion particle to a combination of spins. This is achieved by the Jordan-Wigner (JW) transformation: the creation and annihilation operators acting on the Fock space can be defined as

$$c_l^\dagger = \prod_{j<l} \sigma_j^z \sigma_l^+, \qquad c_l = \prod_{j<l} \sigma_j^z \sigma_l^-, \tag{2.30}$$

where $\sigma^\pm = \frac{\sigma^x \pm i\sigma^y}{2}$, and the operators satisfy the anti-commutation relations

$$\left\{c_l^\dagger, c_n^\dagger\right\} = 0 \qquad \left\{c_l^\dagger, c_n\right\} = \delta_{n,l} \qquad \{c_l, c_n\} = 0. \tag{2.31}$$

One should note that this transformation is a *non-local* transformation. To better understand the above relation, I have opened these relations in appendix B.

As mentioned before because of the string of σ^z, the JW transformation is non-local. However, it does not affect the degrees of freedom enclosed in the subspace $[1, l]$ mapped into the corresponding subspace for both spin and fermionic representations. The non-locality of this transformation affects the terms (interactions) at boundaries. For instance, the open boundary condition means $c_{L+1}^\dagger = 0$ and there is no change from spin to fermion representation. On the other hand, the boundary conditions after the Jordan Wigner transformation, when the chain is periodic, produce:

$$c_{L+1}^\dagger = \hat{\mathcal{N}} c_1^\dagger \tag{2.32}$$

where $\hat{\mathcal{N}} = \prod_{l=1}^{L} \sigma_l^z$ with eigenvalues $\mathcal{N} = \pm 1$. The definition of JW transformation can be understood as associating a spinless quasiparticle to z-spin up in the chain. Then $\hat{\mathcal{N}}$ can be seen as the parity of the spins down or the parity of the number of fermions. In the PBC, (2.32) means that JW transformation puts a product of all σ^z when it passes site L to site 1. This also happens if one uses the inverse JW transformation to get a spin representation of a fermionic model, see appendix C for an example. As it will be elaborated more later, after JW transformation we obtain two chains of fermions, one with normal PBC, and the other with a minus sign when we go around the chain. On the same topic, $\hat{\mathcal{N}}$ commutes with the XY Hamiltonian ($\left[H_{XY}, \hat{\mathcal{N}}\right] = 0$) and divides the Hilbert space into two subspaces, which must be considered separately.

To have a unified notation, we could use the symbol $\mathcal{N}$ for identifying the OBC as well, it means to put $\mathcal{N}^{OBC} = 0$. The Jordan-Wigner transform can be inverted, allowing us to express the Pauli operators in terms of the fermion operators $c_l^\dagger$ and c_l. In particular, we have:

$$\sigma_l^z = c_l^\dagger c_l - c_l c_l^\dagger, \qquad \sigma_l^x = \prod_{j<l} \sigma_j^z (c_l + c_l^\dagger), \qquad \sigma_l^y = i \prod_{j<l} \sigma_j^z (c_l - c_l^\dagger). \tag{2.33}$$

These expressions for σ^x and σ^y are rather inconvenient, involving as they do products of large numbers of Fermi operators. However, for certain simple products of Pauli operators, it is possible to obtain simple expressions in terms of the Fermi operators. In particular, with a little algebra we see that:

$$\sigma_l^x \sigma_{l+1}^x = -(c_l^\dagger - c_l)(c_{l+1} + c_{l+1}^\dagger)$$

Here, we do not go through the fermionization calculations part by part, you can refer to appendix B. Putting all the relations (2.33) together with Hamiltonian (2.2), the fermion version of the XY Hamiltonian is given as follows:

$$H_{XY}(c^\dagger, c) = \frac{J}{2}\sum_{l=1}^{L-1}\left(c_l^\dagger c_{l+1} + \gamma c_l^\dagger c_{l+1}^\dagger + c_{l+1}^\dagger c_l + \gamma c_{l+1} c_l\right) - \frac{J\hat{\mathcal{N}}}{2}\left(c_L^\dagger c_1 - c_L c_1^\dagger + \gamma c_L^\dagger c_1^\dagger - \gamma c_L c_1\right) - h\sum_{l=1}^{L} c_l^\dagger c_l + \frac{hL}{2} \tag{2.34}$$

Now, the XY Hamiltonian is made from pair of fermion creation and annihilation operators, which is also the reason to name it *Quadratic fermion* model. These models are also known as free fermion models since there are no fermion-fermion interactions in the Hamiltonian above. It should be emphasized that starting from a PBC spin chain (2.2), we obtained two versions of the PBC free fermion model, one with PBC ($\mathcal{N} = -1$) and the other with anti-periodic boundary condition ($\mathcal{N} = +1$).

It will be clear later that the Hamiltonian (2.34) having a quadratic form in the fermionic creation and annihilation operators is essential: the Hamiltonian can be diagonalized exactly (numerical or analytical), see section 2.3.2. Additionally, the expectation value of any n-point and/or complex function of these operators can be calculated with respect to the expectation values of 2-point fermionic operators (Wick theorem [50]). The following section addresses the study and diagonalization of quadratic fermion Hamiltonians such as (2.34), and even more general quadratic fermion Hamiltonians. A more detailed diagonalization process for open and periodic boundary conditions is presented in the following parts of this thesis. Intriguingly, in 1D, any quadratic fermion Hamiltonian can be written in Majorana form [51] and it is discussed later in this chapter. The ground state or any state in the spectrum of XY model (2.2) can be obtained by correct projection of eigenstates of diagonalized fermionic Hamiltonian. A comprehensive discussion on the location of the spin chain can be found in section 2.4.3.

2.3 Quadratic fermions model

In this part, we want to study the general quadratic fermionic models. In particular, we study the general properties of these models and the means to diagonalize the Hamiltonian. Due to the quadratic form of Hamiltonian These systems are also called free fermions. The interest in free-fermion systems is because while still exactly solvable, certain quadratic Hamiltonians are good approximations for more complicated systems, like e.g. the BCS-Hamiltonian used in the theory of superconductivity. Unlike the spin chain studies presented before, the material in this section is valid for any dimension and not just the 1D. The diagonalization process is discussed for open and (anti)periodic boundary conditions. In this section, we study some particular states and discuss their characteristics. One can find the correlation matrices, density matrix formulation and the entanglement of these systems in chapters 3, 4 and 5.

2.3.1 General properties

The Hamiltonian of general free quadratic fremions can be written as:

$$H = \sum_{i,j=1}^{L} \left[c_i^\dagger A_{ij} c_j + \tfrac{1}{2} c_i^\dagger B_{ij} c_j^\dagger + \frac{1}{2} c_i B_{ji}^* c_j \right] - \frac{1}{2}\mathrm{tr}(\mathbf{A}^*) \tag{2.35}$$

where L is the number of sites. Here, the matrix $\mathbf{A}$ is Hermitian, $\mathbf{A} = \mathbf{A}^\dagger$ and the $\mathbf{B}$ matrix is anti-symmetric (skew-symmetric), $\mathbf{B} = -\mathbf{B}^T$. we can write the Hamiltonian (2.35) in a more compact matrix notation as:

$$H = \frac{1}{2} \begin{pmatrix} \mathbf{c}^\dagger & \mathbf{c} \end{pmatrix} \mathbf{M} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix}, \qquad \text{where} \quad \mathbf{M} = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B}^* & -\mathbf{A}^* \end{pmatrix}, \tag{2.36}$$

and $\mathbf{c}^{(\dagger)}$ is the column/row of fermionic creation and annihilation operators,

$$\mathbf{c}^{(\dagger)} = \begin{pmatrix} c_1^{(\dagger)} \\ c_2^{(\dagger)} \\ \vdots \\ c_L^{(\dagger)} \end{pmatrix}. \tag{2.37}$$

The fermion operators above (c, $c^\dagger$) are known as Dirac fermions.

It is useful to write the Hamiltonian in terms of Majorana fermions, as they are widely used in the condensed matter and quantum many-body literature. Majorana fermions can be written in terms of c-fermions (defined before) as:

$$\gamma_j = c_j + c_j^\dagger, \qquad \bar{\gamma}_j = i(c_j^\dagger - c_j). \tag{2.38}$$

Most of the calculations are easier and more compact in the Majorana representation. Consider the generic Hamiltonian (2.35), one can write the Hamiltonian in the Majorana

representation as:

$$H = \frac{1}{4}(\boldsymbol{\gamma}\ \bar{\boldsymbol{\gamma}})\mathbf{W}\begin{pmatrix}\boldsymbol{\gamma}\\ \bar{\boldsymbol{\gamma}}\end{pmatrix}, \tag{2.39}$$

$$\mathbf{W} = \begin{pmatrix}\mathbf{A}_a+\mathbf{B}_s & i(\mathbf{B}_a+\mathbf{A}_s)\\ i(\mathbf{B}_a-\mathbf{A}_s) & \mathbf{A}_a-\mathbf{B}_s\end{pmatrix}, \tag{2.40}$$

where $\mathbf{A}_{s(a)} = \frac{\mathbf{A}\pm\mathbf{A}^T}{2}$ and $\mathbf{B}_{s(a)} = \frac{\mathbf{B}^\dagger\pm\mathbf{B}}{2}$, which stand for symmetric and anti-symmetric combination of $\mathbf{A}$ (and $\mathbf{B}$). Note that $\mathbf{A}^*_{s(a)} = \pm\mathbf{A}_{s(a)}$ and $\mathbf{B}^*_{a(s)} = \pm\mathbf{B}_{a(s)}$, meaning that the $\mathbf{W}$ matrix is purely imaginary antisymmetric matrix (consequently Hermitian). In chapter 3, we mostly calculate the correlation functions for Majorana fermions rather than Dirac fermions.

The eigenstates of the quadratic Hamiltonian (2.35) are eigenstates of the parity operator too which means that Hamiltonian commutes with the parity. The parity operator is given by

$$P = (-1)^{\sum n_i} = \prod_{i=1}^{L}(1-2c_i^\dagger c_i) \tag{2.41}$$

where n_i is number of fermions at site i and $\sum n_i$ is the total number of fermions. Above can be written as:

$$P = e^{i\frac{\pi L}{2}} e^{\frac{i\pi}{2}(\mathbf{c}^\dagger\ \mathbf{c})\begin{pmatrix}\mathbf{I} & 0\\ 0 & -\mathbf{I}\end{pmatrix}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^\dagger\end{pmatrix}}, \tag{2.42}$$

and then we have

$$P^{-1}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^\dagger\end{pmatrix}P = -\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^\dagger\end{pmatrix}. \tag{2.43}$$

Using the above equation we can easily show that $P^{-1}HP = H$.

2.3.2 Diagonalization

To find the spectrum and energy level of free fermionic Hamiltonians, we need to find eigenvalues of the matrix $\mathbf{H}$. These matrices grow exponentially with the size of the system, which makes it extremely difficult to find their eigenvalues. In this part, we are going to present analytical or easy computational methods to find the spectrum of the given Hamiltonian. For instance, we can diagonalize the (2.36) using Unitary transformation and write

$$H = \frac{1}{2}\begin{pmatrix}\mathbf{c}^\dagger & \mathbf{c}\end{pmatrix}\mathbf{U}^\dagger\mathbf{U}\mathbf{M}\mathbf{U}^\dagger\mathbf{U}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^\dagger\end{pmatrix} = \frac{1}{2}\begin{pmatrix}\eta^\dagger & \eta\end{pmatrix}\begin{pmatrix}\mathbf{\Lambda} & 0\\ 0 & -\mathbf{\Lambda}\end{pmatrix}\begin{pmatrix}\eta\\ \eta^\dagger\end{pmatrix}, \tag{2.44}$$

where $\begin{pmatrix}\eta\\ \eta^\dagger\end{pmatrix} = \mathbf{U}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^\dagger\end{pmatrix}$ is the new quasiparticle. The $\eta^{(\dagger)}$ is not an actual particle and the Hamiltonian matrix has a diagonal form in the basis of this new quasiparticle. The

$\mathbf{\Lambda}$ is diagonal matrix with non-negative elements λ_k. The components of this diagonal matrix are the energy modes of quasiparticles and the spectrum of the Hamiltonian is made from the activation (or annihilation) of different modes. Therefore, the diagonal form of Hamiltonian (2.35) is:

$$H = \sum_k \lambda_k \eta_k^\dagger \eta_k - \frac{1}{2}\mathrm{tr}(\mathbf{\Lambda}). \tag{2.45}$$

The vacuum state $|0\rangle$ is the state which annihilates by all the η_k's,

$$\eta_k |0\rangle = 0, \tag{2.46}$$

for all k.

Now, we seek to find the eigenstates of the Hamiltonian and it is a necessity to have some selection rules for later use. Therefore, we start by introducing the operator J as [52]:

$$\mathbf{J}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} v^* \\ u^* \end{pmatrix}. \tag{2.47}$$

We can show that this operator anticommutes with matrix $\mathbf{M}$ (2.36) in a way that

$$\big(\mathbf{MJ} + \mathbf{JM}\big)\begin{pmatrix} u \\ v \end{pmatrix} = 0. \tag{2.48}$$

To verify the relation above, we start by:

$$\mathbf{MJ}\begin{pmatrix} u \\ v \end{pmatrix} = \mathbf{M}\begin{pmatrix} v^* \\ u^* \end{pmatrix} = \begin{pmatrix} \tilde{\mathbf{A}}v^* + \tilde{\mathbf{B}}u^* \\ -\tilde{\mathbf{B}}^*u^* - \tilde{\mathbf{A}}^*v^* \end{pmatrix} = \mathbf{J}\begin{pmatrix} -\tilde{\mathbf{B}}u - \tilde{\mathbf{A}}v \\ \tilde{\mathbf{A}}^*v + \tilde{\mathbf{B}}^*u \end{pmatrix} = -\mathbf{JM}\begin{pmatrix} u \\ v \end{pmatrix}.$$

As consequence, if $\begin{pmatrix} u \\ v \end{pmatrix}$ is an eigenvector of Hamiltonian with eigenvalue λ then the vector $\mathbf{J}\begin{pmatrix} u \\ v \end{pmatrix}$ is an eigenvector with eigenvalue $-\lambda$. It means that one does not need to find all the eigenstates of Hamiltonian. Finding the eigenstates corresponding to positive eigenvalues is enough. We can get the eigenstates for negative eigenvalue by acting on positive eigenstates with $\mathbf{J}$. Now, going back to transformations that diagonalize Hamiltonian as in (2.44), we know that the $\mathbf{U}$ should have the form

$$\mathbf{U} = \begin{pmatrix} g & h \\ h^* & g^* \end{pmatrix}, \tag{2.49}$$

which also can be written as

$$\mathbf{U} = \begin{pmatrix} u \\ \mathbf{J}u \end{pmatrix}, \qquad \text{where} \qquad u = \begin{pmatrix} \mathbf{g} & \mathbf{h} \end{pmatrix}. \tag{2.50}$$

To complete the diagonalization procedure, we can write for η's operators:

$$\eta_k = \sum_{j=1}^{L} g_{kj} c_j + h_{kj} c_j^\dagger, \qquad \eta_k^\dagger = \sum_{j=1}^{L} h_{kj}^* c_j + g_{kj}^* c_j^\dagger. \tag{2.51}$$

From the inverse transformation, we can write the c-fermions in terms η-operators as:

$$c_k = \sum_{j=1}^{L} (g_{j,k}^* \eta_j + h_{j,k} \eta_j^\dagger), \qquad c_k^\dagger = \sum_{j=1}^{L} (h_{jk}^* \eta_j + g_{jk} \eta_j^\dagger). \tag{2.52}$$

The c-fermions are also known as the real space operators while the η ones are defined in other space connected to real one with the transformation $\mathbf{U}$.

The diagonalizing transformation (matrix $\mathbf{U}$) could be obtained either analytically or by exact numeric diagonalization of $\mathbf{M}$, based on the specific model at the hand. In the section 2.4, I go through more details of the solving the Hamiltonian (2.2) which is related to the Hamiltonian (2.35) (only next nearest interactions) with periodic and open boundary conditions. Some of the analytical calculations in diagonalization of XY spin chain can be extended to a general form of free fermions. In the following part, a different representation of the fermionic vacuum (ground state) is presented. The new formulation of vacuum is very useful in the calculation of reduced density matrix, chapter 4, and calculation of entanglement, chapter 5.

2.3.3 Etta's Vacuum in the configuration basis

We have already introduced the unitary transformation that diagonalizes the Hamiltonian (2.35). In this subsection, we talk about the vacuum of η-operators because computationally this state is more important than the rest, and also there are many technicalities in finding this state. In the rest of this subsection, we introduce different methods to calculate the vacuum of η. Computationally, we can find a matrix representation for Hamiltonian and fermionic operators which satisfies the algebra (commutation or anti-commutation). Having this in mind, we could find the form of the vacuum. The process of finding such a state is fairly straightforward, one needs to find the state in which $\eta_k |0\rangle = 0$ for all $k \in \{1, \cdots, L\}$. The next step is to fix L and find the solution for a general state for each size.

Using the methods above, it is not easy to find the vacuum of η for a large size L. In that method, the number of equations needed to be solved increases exponentially. Also due to the possible degeneracy in the spectrum of the system, it would not be trivial to select the vacuum. There is another method that is much more efficient to get the vacuum in exponential form. Having the desired state in the exponential form helps us to study the entanglement more efficiently (see section 4.1). One can write the vacuum of η, $|0\rangle_\eta$, in terms of the vacuum state of the c-fermions $|0\rangle_c$ [13]. If the parity of $|0\rangle_c$ is positive

then we have:

$$|0\rangle_\eta = \frac{1}{\Big(\det[\mathbf{I}+\mathbf{R}^\dagger\mathbf{R}]\Big)^{\frac{1}{4}}} e^{\frac{1}{2}\sum_{i,j} R_{ij}c_i^\dagger c_j^\dagger}\,|0\rangle_c \tag{2.53}$$

where $c_j\,|0\rangle_c = 0$ for all j and $\mathbf{R}$ is an antisymmetric matrix, using the $\eta_k\,|0\rangle = 0$ we can show that

$$\mathbf{g}.\mathbf{R} + \mathbf{h} = 0. \tag{2.54}$$

It should be pointed out that we can find a solution for the $\mathbf{R}$ matrix if the $\mathbf{g}$ is invertible. There is no guarantee that the $\mathbf{g}$ of the particular system has an inverse. However, one can find a canonical transformation that makes the $\mathbf{g}$ invertible and does not change the parity of vacuum [53]. For instance, such a transformation could be the following change

$$\left.\begin{array}{llll} c_j \;\to\; \tilde{c}_j^\dagger, & & c_j^\dagger \;\to\; \tilde{c}_j \\ c_k \;\to\; \tilde{c}_k^\dagger, & & c_k^\dagger \;\to\; \tilde{c}_k \end{array}\right\} \quad \text{for even number of fermion operators} \tag{2.55}$$

We call this transformation *Tilda transformation*. This transformation does not change the underlying algebra of the system.

In the case where the vacuum has parity $P_0 = -1$, we would not be able to use the equation (2.53). The parity of vacuum is equal to $\det[\mathbf{U}]$. To use the equation above one needs to do a canonical transformation (Tilda transformation), as before, to change the parity of the ground state of c-fermions.

$$c_j \;\to\; \tilde{c}_j^\dagger \qquad \text{and} \qquad c_j^\dagger \;\to\; \tilde{c}_j \tag{2.56}$$

for **only one** specific index j (if we choose $j = 1$ then this transformation can be written as $\widetilde{\mathcal{P}} = e^{i\frac{\pi}{2}\sigma_1^x}$). If as in the previous case the $\mathbf{g}$ is not invertible, then we could use this transformation for an odd number of fermions. With the following transformation, we could use the $|0\rangle_c$ and we would get the right parity for the vacuum. To put in another word, after the following transformation $\det[\tilde{\mathbf{U}}] = +1$, and we have:

$$\widetilde{H} = \frac{1}{2}\begin{pmatrix} \tilde{\mathbf{c}}^\dagger & \tilde{\mathbf{c}} \end{pmatrix} \widetilde{\mathbf{M}} \begin{pmatrix} \tilde{\mathbf{c}} \\ \tilde{\mathbf{c}}^\dagger \end{pmatrix}, \quad \text{where} \quad \widetilde{\mathbf{M}} = \begin{pmatrix} \widetilde{\mathbf{A}} & \widetilde{\mathbf{B}} \\ -\widetilde{\mathbf{B}}^* & -\widetilde{\mathbf{A}}^* \end{pmatrix}. \tag{2.57}$$

The matrices $\widetilde{\mathbf{A}}$ and $\widetilde{\mathbf{B}}$ are very similar to the forms of equations (7.8). The difference is that the first row and columns have different signs. We can also address the unitary transformation which diagonalizes the Hamiltonian (2.57).

$$\widetilde{H} = \frac{1}{2}\begin{pmatrix} \tilde{\mathbf{c}}^\dagger & \tilde{\mathbf{c}} \end{pmatrix} \widetilde{\mathbf{U}}^\dagger\widetilde{\mathbf{U}}\widetilde{\mathbf{M}}\widetilde{\mathbf{U}}^\dagger\widetilde{\mathbf{U}} \begin{pmatrix} \tilde{\mathbf{c}} \\ \tilde{\mathbf{c}}^\dagger \end{pmatrix} = \frac{1}{2}\begin{pmatrix} \tilde{\eta}^\dagger & \tilde{\eta} \end{pmatrix} \begin{pmatrix} \mathbf{\Lambda} & 0 \\ 0 & -\mathbf{\Lambda} \end{pmatrix} \begin{pmatrix} \tilde{\eta} \\ \tilde{\eta}^\dagger \end{pmatrix},$$

where $\begin{pmatrix} \tilde{\eta} \\ \tilde{\eta}^\dagger \end{pmatrix} = \widetilde{\mathbf{U}} \begin{pmatrix} \tilde{\mathbf{c}} \\ \tilde{\mathbf{c}}^\dagger \end{pmatrix}$. The eigenvalues of Hamiltonian would not be affected after this transformation. Since we are able to select the fermion to make this Tilda transformation,

one can choose to $c_1 \rightarrow \tilde{c}_1^\dagger$ and $c_1^\dagger \rightarrow \tilde{c}_1$. Now we use equation (2.53) to find the vacuum of ηs in terms of the ground state of c fermions. Therefore we have

$$\left|\tilde{0}\right\rangle_\eta = \frac{1}{\left(\det[\mathbf{I}+\widetilde{\mathbf{R}}^\dagger\widetilde{\mathbf{R}}]\right)^{\frac{1}{4}}} e^{\frac{1}{2}\sum_{i,j}\tilde{R}_{ij}\tilde{c}_i^\dagger\tilde{c}_j^\dagger}\left|\tilde{0}\right\rangle_c, \tag{2.58}$$

and $\left|\tilde{0}\right\rangle_c$ is the state annihilated by $\tilde{c}_0$, c_1, c_2 and so on. A note to be made here is that the $\left|\tilde{0}\right\rangle_c = (c_1 + c_1^\dagger)\left|0\right\rangle_c$.

2.3.4 Excited eigenstate in the configuration basis

Previously, we saw that we can write the vacuum of η in terms of the vacuum of c-operators which we used an exponential function of c-fermions. It was important to take care of the parity; The method worked for the even parity vacuum only. Now we want to show that any eigenstate of η's can be written in terms of the vacuum of c's with an exponential function. It makes sense, for translational invariant free fermions we know that every excited eigenstate is a ground state of another Hamiltonian, which they commute [16].

Excited states can be created by exciting different modes on the vacuum. This is achieved by acting with different $\eta^\dagger$-operators on the vacuum (2.46).

$$\left|\psi\right\rangle = \left|k_1, k_2, \cdots, k_N\right\rangle = \prod_{k_j\in\mathbb{E}} \eta_{k_j}^\dagger \left|0\right\rangle, \qquad E_\psi = \sum_{k_j\in\mathbb{E}} k_j \tag{2.59}$$

where set $\mathbb{E}$ could be any subset of modes. the states created above are called excited eigenstates of Hamiltonian. We denote the set of indexes of excited modes as $\mathbb{E}$ and the set of modes that are not excited as $\bar{\mathbb{E}}$. We assume that we can write the following excited state in the exponential form as [13]:

$$\left|\psi\right\rangle = C^\psi e^{\frac{1}{2}\sum_{i,j} R_{ij}^\psi c_i^\dagger c_j^\dagger}\left|0\right\rangle_c \tag{2.60}$$

where $C^\psi = \frac{1}{\sqrt[4]{\det[\mathbf{I}+\mathbf{R}^{\psi\,\dagger}\mathbf{R}^\psi]}}$. For this excited state we have:

$$\begin{aligned} \eta_{k_j}\left|\psi\right\rangle &= 0; \qquad k_j \in \bar{\mathbb{E}} \\ \eta_{k_n}^\dagger\left|\psi\right\rangle &= 0; \qquad k_n \in \mathbb{E} \end{aligned} \tag{2.61}$$

Now to find the $\boldsymbol{R}^\psi$ for an excited state, we use the results above and write the η in terms of c using equation (2.51).

$$\begin{aligned} \eta_{k_j}\left|\psi\right\rangle =& C^\psi(g_{k_j l}c_l + h_{k_j l}c_l^\dagger)e^{\frac{1}{2}R_{nm}^\psi c_n^\dagger c_m^\dagger}\left|0\right\rangle_c = Ne^{\frac{1}{2}R_{nm}^\psi c_n^\dagger c_m^\dagger}\Big[g_{k_j l}(\frac{R_{lm}^\psi}{2}c_m^\dagger - \frac{R_{nl}^\psi}{2}c_n^\dagger) + h_{k_j l}c_l^\dagger\Big]\left|0\right\rangle_c \\ =& C^\psi e^{\frac{1}{2}R_{nm}^\psi c_n^\dagger c_m^\dagger}\Big[g_{k_j l}R_{lm}^\psi + h_{k_j m}\Big]c_m^\dagger\left|0\right\rangle_c = 0; \qquad k_j \in \bar{\mathbb{E}} \end{aligned}$$

Therefore

$$g_{k_j l}R_{lm}^\psi + h_{k_j m} = 0; \qquad k_j \in \bar{\mathbb{E}}. \tag{2.62}$$

From the second line of equation (2.61) we get:

$$h^*_{k_n l} R^{\psi}_{lm} + g^*_{k_n m} = 0; \qquad k_n \in \mathbb{E}. \tag{2.63}$$

We have found the $\boldsymbol{R}^{\psi}$ for excited state with equation (2.62) and (2.63). We can write a generalized formula for the $\boldsymbol{R}^{\psi}$ as

$$\mathfrak{g}\boldsymbol{R}^{\psi} + \mathfrak{h} = 0 \tag{2.64}$$

where $\mathfrak{g}$ and $\mathfrak{h}$ are a generalized version of $\mathbf{g}$ and $\mathbf{h}$ given by

$$\mathfrak{g}_{nm} = \begin{cases} g_{nm} & if\ n \in \bar{\mathbb{E}} \\ h^*_{nm} & if\ n \in \mathbb{E} \end{cases} \qquad \mathfrak{h}_{nm} = \begin{cases} h_{nm} & if\ n \in \bar{\mathbb{E}} \\ g^*_{nm} & if\ n \in \mathbb{E} \end{cases} \tag{2.65}$$

Also, same as the section 2.3.3, one should make sure that the $\mathfrak{g}$ has an inverse. If not one should use the canonical (Tilda) transformation to overcome the inversion problem. If applicable, the equation (2.60) gives the excited eigenstate in an exponential form which as remarked before is advantageous in the study of entanglement (see section 4.1).

There is also another method to write the excited eigenstates which do not need the inversion of $\mathbf{g}$ matrix. In this method, although does not face the non-invertibility of matrices, It is not trivial to write the excited in exponential form (at least for more than one mode excited!). For instance, we have calculated the excited state for some number of modes excited.

One mode:
$$\eta^{\dagger}_{k_1}|0\rangle = C(h^*_{k_1 l} c_l + g^*_{k_1 l} c^{\dagger}_l) e^{\frac{1}{2} R_{ij} c^{\dagger}_i c^{\dagger}_j} |0\rangle_c = C e^{\frac{1}{2} R_{ij} c^{\dagger}_i c^{\dagger}_j} (h^*_{k_1 m} R_{ml} + g^*_{k_1 l}) c^{\dagger}_l |0\rangle_c \tag{2.66}$$

Two modes:
$$\begin{aligned} \eta^{\dagger}_{k_2}\eta^{\dagger}_{k_1}|0\rangle &= C(h^*_{k_2 s} c_s + g^*_{k_2 s} c^{\dagger}_s) e^{\frac{1}{2} R_{ij} c^{\dagger}_i c^{\dagger}_j} (h^*_{k_1 m} R_{ml} + g^*_{k_1 l}) c^{\dagger}_l |0\rangle_c \\ &= C e^{\frac{1}{2} R_{ij} c^{\dagger}_i c^{\dagger}_j} \Big[(h^*_{k_2 n} R_{ns} + g^*_{k_2 n}) c^{\dagger}_n + h^*_{k_2 s} c_s \Big] (h^*_{k_1 m} R_{ml} + g^*_{k_1 l}) c^{\dagger}_l |0\rangle_c \\ &= C e^{\frac{1}{2} R_{ij} c^{\dagger}_i c^{\dagger}_j} \Big[\mathfrak{M}_{k_2 n} \mathfrak{M}_{k_1 l} c^{\dagger}_n c^{\dagger}_l + h^*_{k_2 s} \mathfrak{M}_{k_1 s} \Big] |0\rangle_c \end{aligned} \tag{2.67}$$

Three modes:
$$\begin{aligned} \eta^{\dagger}_{k_3}\eta^{\dagger}_{k_2}\eta^{\dagger}_{k_1}|0\rangle &= C(h^*_{k_3 r} c_r + g^*_{k_3 r} c^{\dagger}_r) e^{\frac{1}{2} R_{ij} c^{\dagger}_i c^{\dagger}_j} \Big[\mathfrak{M}_{k_2 n} \mathfrak{M}_{k_1 l} c^{\dagger}_n c^{\dagger}_l + h^*_{k_2 s} \mathfrak{M}_{k_1 s} \Big] |0\rangle_c \\ &= C e^{\frac{1}{2} R_{ij} c^{\dagger}_i c^{\dagger}_j} \Big[(h^*_{k_3 m} R_{mr} + g^*_{k_3 r}) c^{\dagger}_r + h^*_{k_3 r} c_r \Big] \Big[\mathfrak{M}_{k_2 n} \mathfrak{M}_{k_1 l} c^{\dagger}_n c^{\dagger}_l + h^*_{k_2 s} \mathfrak{M}_{k_1 s} \Big] |0\rangle_c \\ &= C e^{\frac{1}{2} R_{ij} c^{\dagger}_i c^{\dagger}_j} \Big[\prod_{k_j} \mathfrak{M}_{k_j l} c^{\dagger}_l + h^*_{k_3 s} \mathfrak{M}_{k_2 s} \mathfrak{M}_{k_1 n} c^{\dagger}_n - h^*_{k_3 s} \mathfrak{M}_{k_2 n} \mathfrak{M}_{k_1 s} c^{\dagger}_n + h^*_{k_2 s} \mathfrak{M}_{k_1 s} \mathfrak{M}_{k_3 n} c^{\dagger}_n \Big] | \end{aligned} \tag{2.68}$$

$$\begin{aligned}\textbf{Four modes:}\quad \eta^\dagger_{k_4}\cdots\eta^\dagger_{k_1}|0\rangle = Ce^{\frac{1}{2}R_{ij}c_i^\dagger c_j^\dagger}\Big[\Big(\prod_{k_j}\mathfrak{M}_{k_j l}c_l^\dagger\Big) + h^*_{k_4 s}\mathfrak{M}_{k_1 s}\mathfrak{M}_{k_3 n}\mathfrak{M}_{k_2 l}c_n^\dagger c_l^\dagger \\ - h^*_{k_4 s}\mathfrak{M}_{k_2 s}\mathfrak{M}_{k_3 n}\mathfrak{M}_{k_1 l}c_n^\dagger c_l^\dagger + h^*_{k_4 s}\mathfrak{M}_{k_3 s}\mathfrak{M}_{k_2 n}\mathfrak{M}_{k_1 l}c_n^\dagger c_l^\dagger \\ - h^*_{k_3 s}\mathfrak{M}_{k_1 s}\mathfrak{M}_{k_4 n}\mathfrak{M}_{k_2 l}c_n^\dagger c_l^\dagger + h^*_{k_3 s}\mathfrak{M}_{k_2 s}\mathfrak{M}_{k_4 n}\mathfrak{M}_{k_1 l}c_n^\dagger c_l^\dagger \\ + h^*_{k_2 s}\mathfrak{M}_{k_1 s}\mathfrak{M}_{k_4 n}\mathfrak{M}_{k_3 l}c_n^\dagger c_l^\dagger + \mathrm{Pf}[\boldsymbol{\chi}]\Big]|0\rangle_c\end{aligned} \tag{2.69}$$

where $\mathfrak{M} = \mathbf{h}^*\mathbf{R} + \mathbf{g}^*$ and $\boldsymbol{\chi}$ is given by

$$\boldsymbol{\chi} = \begin{pmatrix} 0 & h^*_{k_4 a}\mathfrak{M}_{k_3 a} & h^*_{k_4 a}\mathfrak{M}_{k_2 a} & h^*_{k_4 a}\mathfrak{M}_{k_1 a} \\ -h^*_{k_4 a}\mathfrak{M}_{k_3 a} & 0 & h^*_{k_3 a}\mathfrak{M}_{k_2 a} & h^*_{k_3 a}\mathfrak{M}_{k_1 a} \\ -h^*_{k_4 a}\mathfrak{M}_{k_2 a} & -h^*_{k_3 a}\mathfrak{M}_{k_2 a} & 0 & h^*_{k_2 a}\mathfrak{M}_{k_1 a} \\ -h^*_{k_4 a}\mathfrak{M}_{k_1 a} & -h^*_{k_3 a}\mathfrak{M}_{k_1 a} & -h^*_{k_2 a}\mathfrak{M}_{k_1 a} & 0 \end{pmatrix}. \tag{2.70}$$

Although useful, relations above do not have a compact notation. Previously introduced method appears to be more handy to use.

2.3.5 General state in the configuration basis

Let us extend our studies to a general state $|\varphi\rangle$ defined by

$$|\varphi\rangle = \sum_r a_r\,|E_r\rangle \tag{2.71}$$

where $|E_r\rangle$ are the eigenstates of the Hamiltonian with energy E_r, as defined in (2.59). These types of states do not have the Wick theorem normally, which makes them unfavorable to study. For instance to study their entanglement aspects one needs to work with the density matrix of these states and the density matrix grows exponentially with the size of the system. One should note that a general state like (2.71), is not necessarily an eigenstate of the parity operator. However, based on the context, we can use that $ketE_r$ that have the same parity (even or odd).

2.4 Solving the XY spin chain (Spin chain revisited)

After introducing the XY spin chain in section 2.2 and connecting it to a fermionic model via JW transformation, the diagonalization process and structure of eigenvalues and eigenvectors were shown in section 2.3. Now, the results of the diagonalization of free fermions will be used to solve the original spin model. Here, some analytical results will be established for the PBC where spins only interact with the next-nearest spins. Also, some examples of OBC will be displayed. The notation is quite similar to the reference [39], however, I have made the effort to elaborate more on details. The sections might

appear a little technical, however, they provide a concise background to the fermionic representation of the XY model, which will be useful in the rest of the work.

2.4.1 Periodic boundary conditions

As previously seen, the JW transformation maps the XY spin model (2.2) into a chain of non-interacting spinless fermions. In practice, after this transformation we obtain two copies of a fermionic model, one is periodic ($\mathcal{N}=-1$) and the other is an anti-periodic ($\mathcal{N}=+1$) chain. Periodicity (also called translational invariant) is very useful and allows us to diagonalize the Hamiltonian in the Fourier space [39]. hence it is worth recovering it, or in the other words, we want to get rid of the $\hat{\mathcal{N}}$ in the boundary terms of (2.34). Fortunately, the periodicity can be restored by applying the transformation below for a generic L [54],

$$\bar{c}_l = e^{\frac{i\pi(\mathcal{N}+1)l}{2L}} c_l, \tag{2.72}$$

The transformation above eliminates the $\hat{\mathcal{N}}$ appeared in the Hamiltonian (2.34) as:

$$\bar{c}_{_{L+1}} = e^{\frac{i\pi(\mathcal{N}+1)(L+1)}{2L}} c_{L+1} = -\mathcal{N} e^{\frac{i\pi(-\mathcal{N}-1)}{2L}} c_{L+1} = -\mathcal{N} e^{\frac{i\pi(-\mathcal{N}-1)}{2L}} (-\mathcal{N}) c_1 = \mathcal{N}^2 \bar{c}_1 = \bar{c}_1.$$

However, it breaks the translational symmetry (in the corresponding fermionic space). We can see that by substituting $c_l = e^{-\frac{i\pi(\mathcal{N}+1)l}{2L}} \bar{c}_l$ into the equation (2.34). Therefore, we can combine the boundary terms in the sum on l and re-write the whole thing with one sum, as[1]:

$$H_{XY}(\bar{c}^\dagger, \bar{c}) = \frac{J}{2} \sum_{l=1}^{L} \left(e^{\frac{\pi i(-\mathcal{N}-1)}{2L}} \bar{c}_l^\dagger \bar{c}_{l+1} + \gamma e^{-\frac{\pi i(-\mathcal{N}-1)}{2L}} e^{\frac{\pi i(-\mathcal{N}-1)l}{L}} \bar{c}_l^\dagger \bar{c}_{l+1}^\dagger + \ H.C. \right) - h \sum_{l=1}^{L} \bar{c}_l^\dagger \bar{c}_l + \frac{hL}{2} \tag{2.73}$$

I have used the $e^{-\frac{i\pi(\mathcal{N}+1)}{2}} = -\mathcal{N}$ in the boundary terms above knowing $\mathcal{N}^2 = 1$. With the form above, we are able to do Fourier transform. The discrete Fourier transform is defined as: $\bar{c}_l = \frac{1}{\sqrt{L}} \sum_{k=1}^{L} e^{\frac{2i\pi kl}{L}} \tilde{c}_k$, and the Hamiltonian (2.73) will be block-diagonal afterward. To prove this, I substitute the Fourier form of $\bar{c}_l$ in to equation (2.73).The summation on l simplifies to the delta function, $\delta_{k,k'} = \frac{1}{L} \sum_{l=1}^{L} e^{\frac{2i\pi(k'-k)l}{L}}$. With that in mind, we can use this definition of delta function to simplify the rest of the terms and drop the sum on k', Therefore,

$$\begin{aligned} H_{XY}(\tilde{c}^\dagger, \tilde{c}) = & \frac{J}{2} \sum_{k=1}^{L} \Big(e^{\frac{2i\pi k}{L} - \frac{i\pi(\mathcal{N}+1)}{2L}} \tilde{c}_k^\dagger \tilde{c}_k + \gamma e^{-\frac{i\pi(\mathcal{N}+1)}{2L} + \frac{2i\pi k}{L}} \tilde{c}_k^\dagger \tilde{c}_{\frac{\mathcal{N}+1}{2}-k}^\dagger \\ & + e^{\frac{i\pi(\mathcal{N}+1)}{2L} - \frac{2i\pi k}{L}} \tilde{c}_k^\dagger \tilde{c}_k + \gamma e^{+\frac{i\pi(\mathcal{N}+1)}{2L} - \frac{2i\pi k}{L}} \tilde{c}_k \tilde{c}_{\frac{\mathcal{N}+1}{2}-k} \Big) - h \sum_{k=1}^{L} \tilde{c}_k^\dagger \tilde{c}_k + \frac{hL}{2} \end{aligned}$$

[1] It should be mentioned that we concluded this proof for $h=0$. The reason is this part of Hamiltonian is easy to verify under such a transformation.

To simplify further, let us define a new parameter $\phi_k = \frac{2\pi}{L}\left(k - \frac{\mathcal{N}+1}{4}\right)$, and re-wrte the Hamiltonian above, in terms of Fourier creation and annihilation operators $\tilde{c}^\dagger$ and $\tilde{c}$, as:

$$H_{XY}(\tilde{c}^\dagger, \tilde{c}) = \frac{J}{2}\sum_{k=1}^{L}\left(e^{i\phi_k}\tilde{c}_k^\dagger\tilde{c}_k + \gamma e^{+i\phi_k}\tilde{c}_k^\dagger\tilde{c}_{\frac{\mathcal{N}+1}{2}-k}^\dagger + e^{-i\phi_k}\tilde{c}_k^\dagger\tilde{c}_k + \gamma e^{-i\phi_k}\tilde{c}_k\tilde{c}_{\frac{\mathcal{N}+1}{2}-k}\right) - h\sum_{k=1}^{L}\tilde{c}_k^\dagger\tilde{c}_k + \frac{hL}{2}.$$

With the help of Euler formula $e^{i\alpha} = \cos(\alpha) + i\sin(\alpha)$ and the anti-commutation relations $\left\{\tilde{c}_k^{(\dagger)}, \tilde{c}_{k'}^{(\dagger)}\right\} = 0$ and $\left\{\tilde{c}_k^\dagger, \tilde{c}_{k'}\right\} = \delta_{k,k'}$, we can write the above equation as:

$$H_{XY}(\tilde{c}^\dagger, \tilde{c}) = \frac{J}{2}\sum_{k=1}^{L}\left(2\cos(\phi_k)\tilde{c}_k^\dagger\tilde{c}_k + \gamma e^{i\phi_k}\tilde{c}_k^\dagger\tilde{c}_{\frac{\mathcal{N}+1}{2}-k}^\dagger + \gamma e^{-i\phi_k}\tilde{c}_k\tilde{c}_{\frac{\mathcal{N}+1}{2}-k}\right) - h\sum_{k=1}^{L}\tilde{c}_k^\dagger\tilde{c}_k + \frac{hL}{2}. \tag{2.74}$$

Now if we change $k \to -k + \frac{\mathcal{N}+1}{2}$, ϕ_k goes to $-\phi_k$. The reason is that we want to write this Hamiltonian in the simplest form possible (see equation (2.76)). Therefore, let's look at some of the terms above separately. For instance:

$$\sum_k \cos(\phi_k)\tilde{c}_k^\dagger\tilde{c}_k = \frac{1}{2}\sum_k \cos(\phi_k)\left[\tilde{c}_k^\dagger\tilde{c}_k - \tilde{c}_{\frac{\mathcal{N}+1}{2}-k}\tilde{c}_{\frac{\mathcal{N}+1}{2}-k}^\dagger\right] + \frac{1}{2}\sum_k \cos(\phi_k)$$

The last term above vanishes due to sum over all the Fourier modes. It would be the similar for the interaction with external magnetic field term. Putting these calculations together, we can write the Hamiltonian in the matrix form of:

$$H_{XY}(\tilde{c}^\dagger, \tilde{c}) = \sum_k \begin{pmatrix}\tilde{c}_k^\dagger & \tilde{c}_{\frac{\mathcal{N}+1}{2}-k}\end{pmatrix}\frac{1}{2}\begin{pmatrix}J\cos(\phi_k) - h & i\gamma J\sin(\phi_k) \\ -i\gamma J\sin(\phi_k) & -J\cos(\phi_k) + h\end{pmatrix}\begin{pmatrix}\tilde{c}_k \\ \tilde{c}_{\frac{\mathcal{N}+1}{2}-k}^\dagger\end{pmatrix}, \tag{2.75}$$

where $\phi_k = \frac{2\pi}{L}\left(k - \frac{\mathcal{N}+1}{4}\right)$. Then we can write the Hamiltonian in the (block) diagonal form of:

$$H_{XY}^{(\text{PBC})}(\tilde{c}^\dagger, \tilde{c}) = \sum_{k=1}^{L}\begin{pmatrix}\tilde{c}_k^\dagger & \tilde{c}_{\frac{\mathcal{N}+1}{2}-k}\end{pmatrix}\boldsymbol{\mathcal{H}}_k\begin{pmatrix}\tilde{c}_k^\dagger \\ \tilde{c}_{\frac{\mathcal{N}+1}{2}-k}\end{pmatrix}, \tag{2.76}$$

where $\mathcal{H}_k$ is the Hamiltonian restricted to the subspace of the momentas $\frac{2\pi k}{L}$ and $\frac{\pi(\mathcal{N}+1)}{L} - \frac{2\pi k}{L}$ [39]:

$$\mathcal{H}_k = \left[J\cos\left(\frac{2\pi k}{L} - \frac{\pi(\mathcal{N}+1)}{2L}\right) - h\right]\sigma^z - J\gamma\sin\left(\frac{2\pi k}{L} - \frac{\pi(\mathcal{N}+1)}{2L}\right)\sigma^y \tag{2.77}$$

The last step is the Bogolioubov transformation, let us start with the operator relation

$$e^{-i\lambda\hat{B}}\hat{A}e^{i\lambda\hat{B}} = \hat{A} - i\lambda[\hat{B}, \hat{A}] + \cdots + \frac{(-i\lambda)^n}{n!}[\hat{B}, [\hat{B}, [\cdots, [\hat{B}, \hat{A}]\cdots]]] + \cdots, \tag{2.78}$$

which to write the above relation we have used the Taylor expansion for $e^{i\lambda\hat{B}}$. Using above, we can write

$$e^{-i\frac{\theta_k}{2}\sigma^x}\sigma^z e^{i\frac{\theta_k}{2}\sigma^x} = \sigma^z - \theta_k\sigma^y - \frac{\theta_k^2}{2}\sigma^z + \frac{\theta_k^3}{6}\sigma^y + \cdots = \cos\theta_k\sigma^z - \sin\theta_k\sigma^y$$

Using (2.78), I parameterize the $\mathcal{H}_k$ as:

$$\mathcal{H}_k = \lambda_k \, e^{-i\frac{\theta_k}{2}\sigma^x}\sigma^z e^{i\frac{\theta_k}{2}\sigma^x} \tag{2.79}$$

where λ_k is called the dispersion relation and θ_k is called Bogolioubov angle [39]. The explicit relation of the mentioned parameters are given by:

$$\begin{aligned} &\lambda_k = \sqrt{\Big(J\cos\phi_k - h\Big)^2 + J^2\gamma^2\sin^2\phi_k}, && \phi_k = \tfrac{2\pi}{L}\Big(k - \tfrac{\mathcal{N}+1}{4}\Big), \\ &\cos\theta_k = \tfrac{J\cos\phi_k - h}{\lambda_k}, && \sin\theta_k = \tfrac{J\gamma\sin\phi_k}{\lambda_k}. \end{aligned} \tag{2.80}$$

In fact, the Bogolioubov transformation diagonalizes the $\mathcal{H}_k$, and it can be thought of as a rotation in 2×2 subspace of each momentum k. The fermions diagonalizing the Hamiltonian can be obtained by acting on the vector $\begin{pmatrix}\tilde{c}_k^\dagger & \tilde{c}_{-\frac{\mathcal{N}+1}{2}-k}\end{pmatrix}$ with Bogoliubov rotation, for instance:

$$\eta_k^\dagger = \cos(\frac{\theta_k}{2})\tilde{c}_k^\dagger - i\sin(\frac{\theta_k}{2})\tilde{c}_{\frac{\mathcal{N}+1}{4}-k}, \tag{2.81}$$

then

$$H_{XY}(\eta^\dagger,\eta) = \sum_{k=1}^{L}\lambda_k\Big(\eta_k^\dagger\eta_k - \frac{1}{2}\Big) \tag{2.82}$$

This is the diagonal form of the periodic and anti-periodic free fermion Hamiltonian. In comparison to the contents of section 2.3.2, λ_k is the same λ_k introduced in (2.45), for instance, $\sum_{k=1}^{L}\lambda_k = \mathrm{tr}(\boldsymbol{\lambda})$.

As for the transformation $\mathbf{U}$ introduced in section 2.3.2, for PBC (also anti-PBC), we can get the $\mathbf{g}$ and $\mathbf{h}$ matrices analytically. To show this, I fix $\mathcal{N}=-1$ and write the η-fermions in term of c-fermions starting with (2.81):

$$\eta_k^\dagger = \cos(\frac{\theta_k}{2})\tilde{c}_k^\dagger - i\sin(\frac{\theta_k}{2})\tilde{c}_{-k}, \qquad \eta_{-k} = \cos(\frac{\theta_k}{2})\tilde{c}_{-k} - i\sin(\frac{\theta_k}{2})\tilde{c}_k^\dagger. \tag{2.83}$$

As it was mentioned before, for $\mathcal{N}=-1$ sector, we have $\bar{c}_l = c_l$, which allows us to do an inverse Fourier transform to get:

$$\begin{pmatrix}\eta_k^\dagger \\ \eta_{-k}\end{pmatrix} = \frac{1}{L}\sum_{k=1}^{L} e^{\frac{2\pi i k l}{L}} e^{i\frac{\theta_k}{2}\sigma^x}\begin{pmatrix}c_l^\dagger \\ c_l\end{pmatrix}. \tag{2.84}$$

Comparing with the (2.51), we can see that

$$g_{kl} = \frac{1}{L}\sum_{k=1}^{L} e^{\frac{2\pi i k l}{L}}\cos(\frac{\theta_k}{2}) \quad \text{and} \quad h_{kl} = \frac{i}{L}\sum_{k=1}^{L} e^{\frac{2\pi i k l}{L}}\sin(\frac{\theta_k}{2}) \tag{2.85}$$

Now we have been able to find the transformation that diagonalizes our Hamiltonian analytically and it means we can solve it exactly. Although the result above is for the $\mathcal{N}=-1$ only, the analytical calculations for the anti-periodic case should be obtained in the same manner.

For the inverse transformation, From $c_l^{(\dagger)}$ to $\eta_k^{(\dagger)}$, we proceed the same way to drive the equation (2.52). Let us starting by writing the $\tilde{c}_{-k+\frac{\mathcal{N}+1}{2}}$ and $\tilde{c}_k^\dagger$ as a function of η-operators:

$$\begin{pmatrix} \tilde{c}_k^\dagger \\ \\ \tilde{c}_{-k+\frac{\mathcal{N}+1}{4}} \end{pmatrix} = \begin{pmatrix} \cos\frac{\theta_k}{2} & i\sin\frac{\theta_k}{2} \\ \\ i\sin\frac{\theta_k}{2} & \cos\frac{\theta_k}{2} \end{pmatrix} \begin{pmatrix} \eta_k^\dagger \\ \\ \eta_{-k+\frac{\mathcal{N}+1}{4}} \end{pmatrix} = e^{i\frac{\theta_k}{2}\sigma^x} \begin{pmatrix} \eta_k^\dagger \\ \\ \eta_{-k+\frac{\mathcal{N}+1}{4}} \end{pmatrix} \tag{2.86}$$

Putting $\mathcal{N} = -1$, and preforming the inverse Fourier transformation, we can expressing the JW fermions, $\hat{c}^{(\dagger)}$, in terms of the Bogolioubov ones, $\hat{\eta}^{(\dagger)}$, as:

$$\begin{pmatrix} c_l^\dagger \\ c_l \end{pmatrix} = \frac{1}{\sqrt{L}} \sum_{k=1}^{L} e^{-\frac{2\pi i k l}{L}} \begin{pmatrix} \tilde{c}_k^\dagger \\ \tilde{c}_{-k} \end{pmatrix} = \frac{1}{\sqrt{L}} \sum_{k=1}^{L} e^{-\frac{2\pi i k l}{L}} e^{i\frac{\theta_k}{2}\sigma^x} \begin{pmatrix} \eta_k^\dagger \\ \eta_{-k} \end{pmatrix} \tag{2.87}$$

Same as before, we are not going through the calculations for $\mathcal{N} = +1$.

The results of this part can easily be applied to other models in the family of XY-chain, such as Ising or the XX model. The exact expressions for quantities like $\mathbf{g}$, $\mathbf{h}$ and λ_k allow us to calculate entanglement, correlations, and so on, without much effort. In the next subsection, we go over some known results for OBC systems.

2.4.2 Open boundary conditions

In this subsection, we consider the XY model with open boundary conditions. due to the boundaries, the Hamiltonian does not simplify in Fourier transform, like (2.76). Apart from some specific cases, the diagonalization is more complicated. For this reason, we just discuss the easy case, however, considering the more general problem of diagonalizing an OBC quadratic Hamiltonian, a good review can be found in the thesis [39]. The diagonalizing transformations (7.14) can be solved easily in the isotropic case (XX model with $\gamma = 0$), and for $\gamma = \pm 1$ (quantum Ising model). In the following, we only focus on the XX model.

The fermionic version (2.34) of the XX Hamiltonian (2.28) with OBC is:

$$H_{XX}^{\text{OBC}} = \frac{J}{2} \sum_{l=1}^{L-1} \left(c_l^\dagger c_{l+1} + c_{l+1}^\dagger c_l \right) - h \sum_{l=1}^{L} c_l^\dagger c_l + \frac{hL}{2}. \tag{2.88}$$

The number of particles (JW fermions) is conserved in this model, indeed one can write $H_{XX} = \sum_{l,n} c_l^\dagger \mathbf{M}_{l,n} c_n$. This can be solved by diagonalizing the tridiagonal symmetric Toeplitz matrix $\mathbf{M}$. The new fermions (quasiparticles) that diagonalize H_{XX}^{OBC} are given by:

$$\eta_k^\dagger = \sqrt{\frac{2}{L+1}} \sum_{l=1}^{L} \sin\left(\frac{\pi k l}{L+1}\right) c_l^\dagger, \tag{2.89}$$

Comparing to the PBC case, with $\gamma = 0$ in (2.80), the η-fermion is given by:

$$\eta_k^\dagger = \sqrt{\frac{2}{L}} \sum_{l=1}^{L} \sin\left(\frac{\pi k l}{L}\right) c_l^\dagger, \tag{2.90}$$

which is quite similar. It is another example of why the XX model is considered to be the simplest spin model previously in this thesis. The fact is, the XX spin chain has only $\mathbf{A}$ and $\mathbf{B} = 0$, both in OBC and PBC cases. Then diagonalization reduces to solving the Eigen equation of a Toeplitz matrix which can be obtained analytically. Some mathematical reviews can be found in [55, 56].

Substituting the (2.89) into the Hamiltonian (2.88) gives:

$$H_{XX}^{OBC} = \sum_{k=1}^{L} \Big(J\cos(\frac{\pi k}{L+1}) - h \Big) \eta_k^\dagger \eta_k + \frac{hL}{2}, \tag{2.91}$$

which is the diagonal version of OBC XX Hamiltonian. It also gives the energy of modes as:

$$\lambda_k = J\cos(\frac{\pi k}{L+1}) - h. \tag{2.92}$$

Unlike the general XY chain, λ_k^{XX} can be negative. Consequently, the ground state is not the vacuum of the operators η, $|0\rangle$. The ground state is the lowest energy possible which is obtained by exciting all the negative modes,

$$|\mathrm{GS}_{XX}\rangle = \prod_{k_j^*} \eta_{k_j^*}^\dagger \, |0\rangle \, ; \quad \lambda_{k^*} < 0. \tag{2.93}$$

Modes with negative energy belong to the Fermi sea. Annihilation of fermions with negative energy (inside the Fermi sea) are excited states of our spectrum. This means that depending on the annihilated k (inside or outside of Fermi sea), we get:

$$\left\langle \eta_k^\dagger \eta_q \right\rangle = \delta_{k,q} \Theta\Big(h - J\cos(\frac{\pi k}{L+1}) \Big),$$

with $\langle \cdots \rangle$ being the expectation value for the XX ground state. This argument is valid for PBC equally.

Finally, we can write the operators c in terms of the ηs:

$$\begin{aligned} \sum_{k=1}^{L} \sin(\frac{\pi k n}{L+1}) \eta_k^\dagger &= \sqrt{\frac{2}{L+1}} \sum_{l=1}^{L} \sum_{k} \sin(\frac{\pi k n}{L+1}) \sin(\frac{\pi k l}{L+1}) c_l^\dagger \\ &= \sqrt{\frac{2}{L+1}} \sum_{l} \frac{L+1}{2} \delta_{l,n} c_l^\dagger = \sqrt{\frac{L+1}{2}} c_n^\dagger. \end{aligned}$$

Then:

$$c_l^\dagger = \sqrt{\frac{2}{L+1}} \sum_{k=1}^{L} \sin(\frac{\pi k l}{L+1}) \eta_k^\dagger \tag{2.94}$$

where we have used the orthogonality of sin functions.

2.4.3 Spin chain ground state

The last piece of the puzzle is to determine the spectrum of the original spin chain (2.2) from the diagonalized fermion Hamiltonian (2.73). The Hamiltonian (2.73) (and eventually

the diagonal one (2.82)) acts on a Hilbert space of dimension 2^L (for fixed $\mathcal{N} = \pm 1$), but only the eigenstates with the correct value of $\mathcal{N}$ are also eigenstates of the original XY spin Hamiltonian [39]: This means that some eigenstates of the original spin Hamiltonian lie in the Hilbert space of $\mathcal{N} = -1$ ($\mathcal{N} = +1$) final diagonal fermion Hamiltonian. In this section, we name those eigenstates of the fermion model which are eigenstates of the XY model as *real* and those who do not belong to the XY model as *not real* states.

To determine which states are real and which ones are not, as it was mentioned, in any sector, states with the right parity ($\mathcal{N}$) are those which are real. Our objective here is to find a method to extract suitable states after the Bogoliubov transformation. To accomplish that, we can write the parity of any state as

$$\mathcal{N} = \prod_{l=1}^{L} \sigma_l^z = (-1)^{n_f} = (-1)^{\sum_{j=1}^{L} c_j^\dagger c_j} = (-1)^{\sum_{k=1}^{L} \tilde{c}_k^\dagger \tilde{c}_k}, \tag{2.95}$$

where the $n_f = \sum_{j=1}^{L} c_j^\dagger c_j$ is the number of fermions of the particular state and $\mathcal{N}_0$ is the parity of the ground state. For the spin chain ground state we have:$H_{XY} \left|GS^{\pm}\right\rangle = E_g^{\pm} \left|GS^{\pm}\right\rangle$ and the energy of ground state is given by $E_g^{\pm} = 1/2 \sum_{k=1}^{L} \lambda_k$. First, One can find a relation for the vacuum of η-fermions as a function of c-vacuum. Since, the possible values of q are different in each sector, for a general $\mathcal{N}$ we have:

$$\left|0^{\pm}\right\rangle_\eta = \prod_{q>0}^{[L-1]/2} \left(\cos(\frac{\theta_q}{2}) - i \sin(\frac{\theta_q}{2}) \tilde{c}_q^\dagger \tilde{c}_{-q}^\dagger \right) \left|0\right\rangle_c \tag{2.96}$$

where $\tilde{c}_q \left|0\right\rangle_c = 0$ for all $q \in [\pm(1 - \frac{\mathcal{N}+1}{4}), \cdots, \pm(L - \frac{\mathcal{N}+1}{4})]$. It is easy to show that $\eta_q \left|0\right\rangle_\eta = 0$ for all allowed q's. In the relation above, there is an even number of c-fermions, $\mathcal{N}_0 = (-1)^{2n} = 1$ and consequently, only states with an even number of b-fermions have the same parity as $\mathcal{N}_0$. To realize which states appear in the original spin chain we separate two cases, (a) L even and (b) L odd.

Case (a) and $\mathcal{N} = +1$: the counter $q = \pm\frac{1}{2}, \cdots, \pm\frac{2L-1}{2}$ which mean $\varphi_q \in (o, \pi)$. For this values, $\sin(\varphi_k)$ is not zero for all the k's. Parity of $\left|0^{+}\right\rangle_\eta$ is $\hat{\mathcal{N}} \left|0^{+}\right\rangle = + \left|0^{+}\right\rangle$ as it was assumed, also this state has the same parity as $\left|0\right\rangle_c$. Since excited states are created by acting on the ground state as $\eta_q^\dagger \left|0^{+}\right\rangle_\eta$ then only states with an even number of excitation are real states and have the write parity.

Case (a) and $\mathcal{N} = -1$: this time $\varphi_k = \frac{2\pi}{L} k$ and $\sin(\varphi_L) = \sin(\varphi_{\frac{L}{2}}) = 0$. This two modes do not need Bogoliubov transformation (from (2.79) and (2.80)):

$$\frac{1}{2} \eta_{\frac{L}{2}}^\dagger \mathcal{H}_{\frac{L}{2}} \eta_{\frac{L}{2}} = -(\frac{J+h}{2})(2\tilde{c}_{\frac{L}{2}}^\dagger \tilde{c}_{\frac{L}{2}} - 1) \tag{2.97}$$

$$\frac{1}{2} \eta_L^\dagger \mathcal{H}_L \eta_L = (J-h)(2\tilde{c}_L^\dagger \tilde{c}_L - 1) \tag{2.98}$$

Based on the sign of the terms above, we could get a lower energy than just using equation (2.96) and some $\tilde{c}^\dagger$ should be added by hand. In fact, exists 4 possibilities that needs more attention:

- $-\frac{J+h}{2} < 0$ and $J > h$ then $|G^-\rangle_\eta = \tilde{c}^\dagger_{L/2} \prod_{q\neq L,\frac{L}{2}} \left(\cos(\frac{\theta_q}{2}) - i\sin(\frac{\theta_q}{2})\tilde{c}^\dagger_q \tilde{c}^\dagger_{-q}\right)|0\rangle_c$
- $-\frac{J+h}{2} < 0$ and $J < h$ then $|G^-\rangle_\eta = \tilde{c}^\dagger_L \tilde{c}^\dagger_{L/2} \prod_{q\neq L,\frac{L}{2}} \left(\cos(\frac{\theta_q}{2}) - i\sin(\frac{\theta_q}{2})\tilde{c}^\dagger_q \tilde{c}^\dagger_{-q}\right)|0\rangle_c$
- $-\frac{J+h}{2} > 0$ and $J > h$ then $|G^-\rangle_\eta = \prod_{q\neq L,\frac{L}{2}} \left(\cos(\frac{\theta_q}{2}) - i\sin(\frac{\theta_q}{2})\tilde{c}^\dagger_q \tilde{c}^\dagger_{-q}\right)|0\rangle_c$
- $-\frac{J+h}{2} > 0$ and $J < h$ then $|G^-\rangle_\eta = \tilde{c}^\dagger_L \prod_{q\neq L,\frac{L}{2}} \left(\cos(\frac{\theta_q}{2}) - i\sin(\frac{\theta_q}{2})\tilde{c}^\dagger_q \tilde{c}^\dagger_{-q}\right)|0\rangle_c$

The regions above allow us to select the correct ground state of the spin chain. Other real excitations come from exciting even number of modes on the correct ground state.

Case (b) and $\mathcal{N} = +1$: same as before, we should look for values of q which $\sin(\varphi_q) = 0$ and this time it happens at $q = \frac{L+1}{2}$. The energy of this mode is given by:

$$\frac{1}{2}\eta^\dagger_{\frac{L+1}{2}} \mathcal{H}_{\frac{L+1}{2}} \eta_{\frac{L+1}{2}} = -(J+h)(2\tilde{c}^\dagger_{\frac{L+1}{2}} \tilde{c}_{\frac{L+1}{2}} - 1). \tag{2.99}$$

Based on the sign of this mode, we have 2 scenarios:

- $-(J+h) > 0$ then $|G^+\rangle_\eta = \prod_{q\neq\frac{L+1}{2}} \left(\cos(\frac{\theta_q}{2}) - i\sin(\frac{\theta_q}{2})\tilde{c}^\dagger_q \tilde{c}^\dagger_{-q}\right)|0\rangle_c$
- $-(J+h) < 0$ then $|G^+\rangle_\eta = \tilde{c}^\dagger_{\frac{L+1}{2}} \prod_{q\neq\frac{L+1}{2}} \left(\cos(\frac{\theta_q}{2}) - i\sin(\frac{\theta_q}{2})\tilde{c}^\dagger_q \tilde{c}^\dagger_{-q}\right)|0\rangle_c$

Same as before, real excited states come from exciting even number of modes on the correct ground state.

Case (b) and $\mathcal{N} = -1$: for $k = L$, we have:

$$\sin(\varphi_L) = 0, \qquad \frac{1}{2}\eta^\dagger_L \mathcal{H}_L \eta_L = (J-h)(2\tilde{c}^\dagger_L \tilde{c}_L - 1). \tag{2.100}$$

Based on the sign of $J-h$, we have 2 scenarios:

- $J-h > 0$ then $|G^-\rangle_\eta = \prod_{q\neq L} \left(\cos(\frac{\theta_q}{2}) - i\sin(\frac{\theta_q}{2})\tilde{c}^\dagger_q \tilde{c}^\dagger_{-q}\right)|0\rangle_c$
- $J-h < 0$ then $|G^-\rangle_\eta = \tilde{c}^\dagger_L \prod_{q\neq L} \left(\cos(\frac{\theta_q}{2}) - i\sin(\frac{\theta_q}{2})\tilde{c}^\dagger_q \tilde{c}^\dagger_{-q}\right)|0\rangle_c$

Same as before, real excited states come from exciting even number of modes on the correct ground state.

This sums up the search for the real spectrum that we were looking for. For the sake of completeness, we show the selection rules for the size $L = 3$ in the B.

— 3 —

Correlations

3.1 Correlation Matrices

Correlations in quantum manybody systems are vital in measuring many quantities. They are even more fundamental in experimental works. Experimental measurement of a quantity in space (and time) comes from measuring correlation functions. Our measurement of how a quantity of a system system evolves in space (and time) comes from measuring correlation functions. Many scattering experiments directly measure correlation functions, for example by X-rays diffraction one can measure the electron specious density–density correlation in laboratory[57]. In this section, we will provide a methods for computing the correlation functions. We will address the calculation of the correlation matrix for different eigenstates of the system including ground state.

We would only address the correlation function for fermion operators, since spin correlation can be related to fermion ones with an JW transformation. For any n-point correlation function $\langle\phi_1\cdots\phi_n\rangle$, since the model is quadratic, all correlation functions can be expressed in terms of two-point functions using Wick's theorem [50]. Wick's theorem gives the practical rule to express a product of creation and annihilation operators as a sum of expectation value of two. In general form, Wick theorem is written as

$$\langle\phi_1\cdots\phi_n\rangle=\sum_{j=2}^{n}(-1)^j\langle\phi_1\phi_j\rangle\langle\phi_2\cdots\phi_{j-1}\phi_{j+1}\cdots\phi_n\rangle \tag{3.1}$$

where ϕ_j's can be any function of creation and annihilation operators. It is more convenient to calculate the correlation matrices for Majorana fermions, with definitions $\gamma_i=c_i+c_i^\dagger$ and $\bar{\gamma}_i=i(c_i^\dagger-c_i)$ for Majorana fermions. It is useful to write the later two point correlation in a block matrix form denoted by $\mathbf{\Gamma}$ as:

$$\mathbf{\Gamma}=\begin{pmatrix}\langle\boldsymbol{\gamma}\cdot\boldsymbol{\gamma}\rangle-\mathbb{I} & \langle\boldsymbol{\gamma}\cdot\bar{\boldsymbol{\gamma}}\rangle\\ \langle\bar{\boldsymbol{\gamma}}\cdot\boldsymbol{\gamma}\rangle & \langle\bar{\boldsymbol{\gamma}}\cdot\bar{\boldsymbol{\gamma}}\rangle-\mathbb{I}\end{pmatrix}=\begin{pmatrix}\mathbf{K}-\mathbb{I} & -i\mathbf{G}^T\\ i\mathbf{G} & \bar{\mathbf{K}}-\mathbb{I}\end{pmatrix}. \tag{3.2}$$

Above, the expectation values have been written for a generic state. From eq. (3.2), we have define

$$\langle\bar{\gamma}_j\gamma_k\rangle=iG_{jk}, \tag{3.3a}$$

$$\langle\gamma_j\gamma_k\rangle=K_{jk}, \tag{3.3b}$$

$$\langle\bar{\gamma}_j\bar{\gamma}_k\rangle=\bar{K}_{jk}. \tag{3.3c}$$

One can write $\mathbf{G}$, $\mathbf{K}$ and $\bar{\mathbf{K}}$ in terms of correlation matrix of c-operators

$$\begin{aligned}\tfrac{1}{i}\langle\bar{\gamma}_j\gamma_k\rangle=&(c_j^\dagger-c_j)(c_k^\dagger+c_k)=\langle c_j^\dagger c_k\rangle-\langle c_jc_k\rangle+\langle c_j^\dagger c_k^\dagger\rangle-\langle c_jc_k^\dagger\rangle\\ =&\langle c_j^\dagger c_k\rangle-\langle c_jc_k\rangle+\langle c_j^\dagger c_k^\dagger\rangle+\langle c_k^\dagger c_j\rangle-\delta_{jk}\end{aligned}$$

$$\begin{aligned}\langle\gamma_j\gamma_k\rangle =&(c_j^\dagger + c_j)(c_k^\dagger + c_k) = \langle c_j^\dagger c_k\rangle + \langle c_j c_k\rangle + \langle c_j^\dagger c_k^\dagger\rangle + \langle c_j c_k^\dagger\rangle\\ =&\langle c_j^\dagger c_k\rangle + \langle c_j c_k\rangle + \langle c_j^\dagger c_k^\dagger\rangle - \langle c_k^\dagger c_j\rangle + \delta_{jk}\\ -\langle\bar\gamma_j\bar\gamma_k\rangle =&(c_j^\dagger - c_j)(c_k^\dagger - c_k) = -\langle c_j^\dagger c_k\rangle + \langle c_j c_k\rangle + \langle c_j^\dagger c_k^\dagger\rangle - \langle c_j c_k^\dagger\rangle\\ =&-\langle c_j^\dagger c_k\rangle + \langle c_j c_k\rangle + \langle c_j^\dagger c_k^\dagger\rangle + \langle c_k^\dagger c_j\rangle - \delta_{jk}\end{aligned}$$

Hence, we can write

$$\begin{aligned}\mathbf{K} &= \mathbf{F}^\dagger + \mathbf{F} + \mathbf{C} - \mathbf{C}^T + \mathbb{I},\\ \bar{\mathbf{K}} &= -\mathbf{F}^\dagger - \mathbf{F} + \mathbf{C} - \mathbf{C}^T + \mathbb{I},\\ \mathbf{G} &= -\mathbf{F}^\dagger + \mathbf{F} + \mathbf{C} + \mathbf{C}^T - \mathbb{I},\end{aligned} \tag{3.4}$$

where $C_{ij} = \langle c_i^\dagger c_j\rangle$ and $F_{ij} = \langle c_i^\dagger c_j^\dagger\rangle$. The $\mathbf{C}$ is a Hermitian matrix and $\mathbf{F}$ is antisymmetric. The $\mathbf{K}$ and $\bar{\mathbf{K}}$ are hermitian too, additionally, we can conclude that $\mathbf{G}$ is real. Knowing these properties, we can prove that the $\mathbf{\Gamma}$ correlation matrix is Hermitian likewise. For instance

$$\begin{aligned}(\mathbf{K} - \mathbb{1})^* &= \mathbf{F}^T + \mathbf{F}^* + \mathbf{C}^* - \mathbf{C}^\dagger = -\mathbf{F} - \mathbf{F}^\dagger + \mathbf{C}^T - \mathbf{C} = -\mathbf{K} + \mathbb{1},\\ (\bar{\mathbf{K}} - \mathbb{1})^* &= -\mathbf{F}^T - \mathbf{F}^* + \mathbf{C}^* - \mathbf{C}^\dagger = \mathbf{F} + \mathbf{F}^\dagger + \mathbf{C}^T - \mathbf{C} = -\bar{\mathbf{K}} + \mathbb{1},\\ \mathbf{G}^* &= -\mathbf{F}^T + \mathbf{F}^* + \mathbf{C}^* + \mathbf{C}^\dagger - I = \mathbf{F} - \mathbf{F}^\dagger + \mathbf{C}^T + \mathbf{C} - \mathbb{I} = \mathbf{G}.\end{aligned}$$

Therefore, we can realize that $\Gamma_{ij}^* = -\Gamma_{ij}$ which means that $\mathbf{\Gamma}$ is pure imaginary. It would be useful to have the $\mathbf{C}$ and $\mathbf{F}$ in terms of $\mathbf{G}$, $\mathbf{K}$ and $\bar{\mathbf{K}}$

$$\begin{aligned}4\mathbf{C} =&\mathbf{K} + \bar{\mathbf{K}} + \mathbf{G} + \mathbf{G}^\dagger,\\ 4\mathbf{F} =&\mathbf{K} - \bar{\mathbf{K}} + \mathbf{G} - \mathbf{G}^\dagger.\end{aligned} \tag{3.5}$$

In the case where $\mathbf{C}$ and $\mathbf{F}$ are real then $\mathbf{C} - \mathbf{C}^T = 0$ and $\mathbf{F} + \mathbf{F}^\dagger = 0$, from this and equation (3.4), one gets

$$\begin{aligned}\mathbf{K} &= \bar{\mathbf{K}} = \mathbb{1},\\ \mathbf{G} &= 2\mathbf{F} + 2\mathbf{C} - \mathbb{I}.\end{aligned} \tag{3.6}$$

When all the correlation functions are real, then we have:

$$\mathbf{\Gamma} = \begin{pmatrix}\mathbf{0} & -i\mathbf{G}^T\\ i\mathbf{G} & \mathbf{0}\end{pmatrix}, \tag{3.7}$$

which means we need to deal with just one matrix $\mathbf{G}$. For example, when we have a Hamiltonian with real parameters the correlation functions for the ground state are all real and the above equation is true. However, when one deals with dynamical problems we do not have real correlations and one should use the equation (3.2). Since this matrix is purely imaginary skew symmetric matrix the eigenvalues come in pairs of opposite sign $(\nu, -\nu)$.

So far, anything said about the correlation matrices was in the most general case. We did not specify anything about the state of the system which these expectation values

are calculated for. Since, there exist a canonical transformation that diagonalize the Hamiltonian, we can analytically calculate the above expectation values in terms of the eigenstates of η-operators.

3.1.1 Expectations for η's vacuum

Using the notation introduced in eq. (2.44), we write c-operators (or γ-operators) in terms of η's. Then we calculate the correlations for the vacuum of η's. For instance

$$\begin{aligned}\langle c_i^\dagger c_j\rangle &= \langle 0|\,(h_{li}^*\eta_l + g_{ki}\eta_k^\dagger)(g_{mj}^*\eta_m + h_{nj}\eta_n^\dagger)\,|0\rangle = \langle 0|\,h_{li}^*\eta_l h_{nj}\eta_n^\dagger\,|0\rangle = h_{li}^* h_{nj}\delta_{nl} = h_{ni}^* h_{nj},\\ \langle c_i^\dagger c_j^\dagger\rangle &= \langle 0|\,(h_{li}^*\eta_l + g_{ki}\eta_k^\dagger)(h_{mj}^*\eta_m + g_{nj}\eta_n^\dagger)\,|0\rangle = \langle 0|\,h_{li}^*\eta_l g_{nj}\eta_n^\dagger\,|0\rangle = h_{li}^* g_{nj}\delta_{nl} = h_{ni}^* g_{nj}.\end{aligned} \tag{3.8}$$

As a result, we can write $\mathbf{C}^0 = \mathbf{h}^\dagger.\mathbf{h}$ and $\mathbf{F}^0 = \mathbf{h}^\dagger.\mathbf{g}$, where superscript zero stands for expectation values calculated in vacuum. From $\mathbf{U}^\dagger.\mathbf{U} = \mathbb{I}$, we have $\mathbf{g}^T.\mathbf{g}^* + \mathbf{h}^\dagger.\mathbf{h} = \mathbb{I}$. Putting these relations in (3.4), we get

$$\begin{aligned}\mathbf{K}^0 =& \mathbf{g}^\dagger.\mathbf{h} + \mathbf{h}^\dagger.\mathbf{g} + \mathbf{h}^\dagger.\mathbf{h} - \mathbf{h}^T.\mathbf{h}^* + \mathbb{I} = \mathbf{g}^\dagger.\mathbf{h} + \mathbf{h}^\dagger.\mathbf{g} + \mathbf{h}^\dagger.\mathbf{h} - \mathbb{I} + \mathbf{g}^T.\mathbf{g}^* + \mathbb{I}\\ =& \mathbf{g}^\dagger.(\mathbf{h}+\mathbf{g}) + \mathbf{h}^\dagger.(\mathbf{h}+\mathbf{g}) = (\mathbf{h}^\dagger + \mathbf{g}^\dagger).(\mathbf{h}+\mathbf{g}),\end{aligned}$$

$$\begin{aligned}\bar{\mathbf{K}}^0 =& -\mathbf{g}^\dagger.\mathbf{h} - \mathbf{h}^\dagger.\mathbf{g} + \mathbf{h}^\dagger.\mathbf{h} - \mathbf{h}^T.\mathbf{h}^* + \mathbb{I} = -\mathbf{g}^\dagger.\mathbf{h} - \mathbf{h}^\dagger.\mathbf{g} + \mathbf{h}^\dagger.\mathbf{h} - \mathbb{I} + \mathbf{g}^T.\mathbf{g}^* + \mathbb{I}\\ =& -\mathbf{g}^\dagger.(\mathbf{h}-\mathbf{g}) + \mathbf{h}^\dagger.(\mathbf{h}-\mathbf{g}) = (\mathbf{h}^\dagger - \mathbf{g}^\dagger).(\mathbf{h}-\mathbf{g}).\end{aligned}$$

Finally

$$\begin{aligned}\mathbf{G}^0 =& -\mathbf{g}^\dagger.\mathbf{h} + \mathbf{h}^\dagger.\mathbf{g} + \mathbf{h}^\dagger.\mathbf{h} + \mathbf{h}^T.\mathbf{h}^* - \mathbb{I} = -\mathbf{g}^\dagger.\mathbf{h} + \mathbf{h}^\dagger.\mathbf{g} + \mathbf{h}^\dagger.\mathbf{h} + \mathbb{I} - \mathbf{g}^T.\mathbf{g}^* - \mathbb{I}\\ =& -\mathbf{g}^\dagger.(\mathbf{h}+\mathbf{g}) + \mathbf{h}^\dagger.(\mathbf{h}+\mathbf{g}) = (\mathbf{h}^\dagger - \mathbf{g}^\dagger).(\mathbf{h}+\mathbf{g}).\end{aligned}$$

Therefore, for the vacuum of η-operators, we can write the expression (3.4) in terms of elements of $\mathbf{U}$ matrix, which tells us that correlation matrix can be calculated much easier.

$$\begin{aligned}\mathbf{K}^0 =& (\mathbf{h}^\dagger + \mathbf{g}^\dagger).(\mathbf{h}+\mathbf{g}),\\ \bar{\mathbf{K}}^0 =& (\mathbf{h}^\dagger - \mathbf{g}^\dagger).(\mathbf{h}-\mathbf{g}),\\ \mathbf{G}^0 =& (\mathbf{h}^\dagger - \mathbf{g}^\dagger).(\mathbf{h}+\mathbf{g}).\end{aligned} \tag{3.9}$$

From the equation (3.9), we can define $\mathbf{V} = \mathbf{h} + \mathbf{g}$ and $\mathbf{W} = \mathbf{h} - \mathbf{g}$. When $\mathbf{C}$ and $\mathbf{F}$ are real $\mathbf{V}$ and $\mathbf{W}$ are unitary matrices, $\mathbf{V}^\dagger.\mathbf{V} = \mathbf{W}^\dagger.\mathbf{W} = \mathbb{I}$. In the end we can write for the full system

$$\mathbf{G}^0 = \mathbf{W}^\dagger.\mathbf{V}. \tag{3.10}$$

It is also not difficult to show that we have

$$\bar{\mathbf{K}} = \mathbf{G}\mathbf{K}^{-1}\mathbf{G}^\dagger. \tag{3.11}$$

In addition when all the correlations are real one can prove that $\det[\mathbf{G}] = \pm 1$.

The formulation introduced so far relies on knowing the elements or expressions of the transformation (2.49) which diagonalize the Hamiltonian. In most cases this can be found by exact numerical methods. Moreover, since the $\mathbf{M}$ increase linearly with the size of the system, then exact numerical methods are valid for big sizes. To be consistent, in the following subsection, we are going to show some analytical examples of correlation functions calculated for the PBC which we know the expression of the $\mathbf{g}$ and $\mathbf{h}$ matrices. For simplicity we assume that coupling constants are Real then one could use the result of (3.6) and (3.7). Particularly, we are going to look at the a general XY case of model and the XX model.

3.1.1.1 Analytical examples

In the general XY case, to calculate the expectation values in (3.3) in respect to η-fermion vacuum. Assuming that we are working in the case where $\mathcal{N} = -1$ (see also [39]), with the help of (2.87), we write the Majorana fermions in terms of η-fermions:

$$\begin{aligned}\gamma_l =& c_l^\dagger + c_l = \frac{1}{\sqrt{L}}\sum_{k=1}^{L} e^{-\frac{2\pi i k l}{L}}\Big(\cos\frac{\theta_k}{2}\eta_k^\dagger + i\sin\frac{\theta_k}{2}\eta_k^\dagger + \cos\frac{\theta_k}{2}\eta_{-k} + i\sin\frac{\theta_k}{2}\eta_{-k}\Big)\\ =&\frac{1}{\sqrt{L}}\sum_{k=1}^{L} e^{-\frac{2\pi i k l}{L}} e^{i\frac{\theta_k}{2}}\Big(\eta_k^\dagger + \eta_{-k}\Big) = \frac{1}{\sqrt{L}}\sum_{k=1}^{L}\Big(e^{-\frac{2\pi i k l}{L}} e^{i\frac{\theta_k}{2}}\eta_k^\dagger + e^{\frac{2\pi i k l}{L}} e^{-i\frac{\theta_k}{2}}\eta_k\Big)\end{aligned} \tag{3.12}$$

$$\begin{aligned}\bar\gamma_l =& i(c_l^\dagger - c_l) = \frac{i}{\sqrt{L}}\sum_{k=1}^{L} e^{-\frac{2\pi i k l}{L}}\Big(\cos\frac{\theta_k}{2}\eta_k^\dagger + i\sin\frac{\theta_k}{2}\eta_{-k} - \cos\frac{\theta_k}{2}\eta_{-k} - i\sin\frac{\theta_k}{2}\eta_k^\dagger\Big)\\ =&\frac{i}{\sqrt{L}}\sum_{k=1}^{L} e^{-\frac{2\pi i k l}{L}}\Big(e^{-i\frac{\theta_k}{2}}\eta_k^\dagger - e^{i\frac{\theta_k}{2}}\eta_{-k}\Big) = \frac{i}{\sqrt{L}}\sum_{k=1}^{L}\Big(e^{\frac{2\pi i k l}{L}} e^{i\frac{\theta_k}{2}}\eta_k - e^{-\frac{2\pi i k l}{L}} e^{-i\frac{\theta_k}{2}}\eta_k^\dagger\Big).\end{aligned}$$

With these relations, it is easy to find the two point correlation functions of Majorana fermions (as in (3.3))

$$\begin{aligned}\langle\gamma_l\gamma_n\rangle =&\frac{1}{L}\sum_{k,q}\langle\Big(e^{-\frac{2\pi i k l}{L}} e^{i\frac{\theta_k}{2}}\eta_k^\dagger + e^{\frac{2\pi i k l}{L}} e^{-i\frac{\theta_k}{2}}\eta_k\Big)\Big(e^{-\frac{2\pi i q n}{L}} e^{i\frac{\theta_q}{2}}\eta_q^\dagger + e^{\frac{2\pi i q n}{L}} e^{-i\frac{\theta_q}{2}}\eta_q\Big)\rangle\\ =&\frac{1}{L}\sum_{k,q} e^{-\frac{2\pi i(qn-kl)}{L}} e^{i\frac{\theta_q-\theta_k}{2}}\langle\eta_k\eta_q^\dagger\rangle = \frac{1}{L}\sum_{k,q} e^{-\frac{2\pi i(qn-kl)}{L}} e^{i\frac{\theta_q-\theta_k}{2}}\delta_{k,q}\\ =&\frac{1}{L}\sum_{k} e^{\frac{2\pi i k(l-n)}{L}} = \delta_{l,n} = \langle\bar\gamma_l\bar\gamma_n\rangle,\end{aligned}$$

which is the same as the results as (3.6). For off-diagonal blocks of $\mathbf{\Gamma}$ we have:

$$\begin{aligned}\langle\gamma_l\bar\gamma_n\rangle =&\frac{i}{L}\sum_{k,q}\langle\Big(e^{-\frac{2\pi i k l}{L}} e^{i\frac{\theta_k}{2}}\eta_k^\dagger + e^{\frac{2\pi i k l}{L}} e^{-i\frac{\theta_k}{2}}\eta_k\Big)\Big(e^{\frac{2\pi i q n}{L}} e^{i\frac{\theta_q}{2}}\eta_q - e^{-\frac{2\pi i q n}{L}} e^{-i\frac{\theta_q}{2}}\eta_q^\dagger\Big)\rangle\\ =&-\frac{i}{L}\sum_{k,q} e^{\frac{2\pi i(kl-qn)}{L}} e^{-i\frac{\theta_q+\theta_k}{2}}\langle\eta_k\eta_q^\dagger\rangle = -\frac{i}{L}\sum_{k,q} e^{\frac{2\pi i(kl-qn)}{L}} e^{-i\frac{\theta_q+\theta_k}{2}}\delta_{k,q}\\ =&-\frac{i}{L}\sum_{k} e^{\frac{2\pi i k(l-n)}{L} - i\theta_k} = -ig_{l,n},\end{aligned}$$

$$\begin{aligned}\langle\bar{\gamma}_l\gamma_n^x\rangle =&\frac{i}{L}\sum_{k,q}\langle\Big(e^{\frac{2\pi ikl}{L}}e^{i\frac{\theta_k}{2}}\eta_k - e^{-\frac{2\pi ikl}{L}}e^{-i\frac{\theta_k}{2}}\eta_k^\dagger\Big)\Big(e^{-\frac{2\pi iqn}{L}}e^{i\frac{\theta_q}{2}}\eta_q^\dagger + e^{\frac{2\pi iqn}{L}}e^{-i\frac{\theta_q}{2}}\eta_q\Big)\rangle\\ =&\frac{i}{L}\sum_{k,q}e^{\frac{2\pi i(kl-qn)}{L}}e^{i\frac{\theta_q+\theta_k}{2}}\langle\eta_k\eta_q^\dagger\rangle = \frac{i}{L}\sum_{k,q}e^{\frac{2\pi i(kl-qn)}{L}}e^{i\frac{\theta_q+\theta_k}{2}}\delta_{k,q}\\ =&\frac{i}{L}\sum_{k}e^{\frac{2\pi ik(l-n)}{L}+i\theta_k}\overset{k\to -k}{=}\frac{i}{L}\sum_{k}e^{\frac{2\pi ik(n-l)}{L}-i\theta_k} = ig_{n,l},\end{aligned}$$

Therefore, we can put everything to gether to get:

$$\mathbf{\Gamma} = \langle\begin{pmatrix}\boldsymbol{\gamma}\\ \bar{\boldsymbol{\gamma}}\end{pmatrix}\begin{pmatrix}\boldsymbol{\gamma} & \bar{\boldsymbol{\gamma}}\end{pmatrix}\rangle - \mathbf{1} = \begin{pmatrix}0 & -i\mathbf{G}^T\\ i\mathbf{G} & \mathbf{0}\end{pmatrix}$$

with

$$G_{l,n} = \frac{1}{L}\sum_{k=1}^{L}e^{\frac{2\pi ik(l-n)}{L}-i\theta_k}.$$

Analytical results for XX chain has a very simple form, as it was explained in chapter 2. In fact the $\mathbf{h}$, introduced in (2.49), is zero for this model, same as the matrix $\mathbf{B}$ of (2.36). It also means that the $\mathbf{F}$ correlation does not exists anymore. Consequently:

$$\mathbf{K} = \bar{\mathbf{K}} = \mathbb{1}, \quad \mathbf{G} = 2\mathbf{C} - \mathbb{I}, \tag{3.13}$$

which also means we can work only with the $\mathbf{C} = \langle GS_{XX}|\, c^\dagger c\,|GS_{XX}\rangle$ correlation.

In the periodic chain of fermions in its ground state, We use the results of correlation functions explained before (in previous example also in [39]) to obtain the correlation matrix C with respect to ground state,

$$\begin{aligned}\left\langle c_l^\dagger c_n\right\rangle =&\delta_{l,n} - \left\langle c_n c_l^\dagger\right\rangle = \frac{1}{L}\sum_k e^{-\frac{2\pi ik}{L}(l-n)}\Big(1-\cos^2(\frac{\theta_k}{2})\Big) = \frac{1}{L}\sum_k e^{-\frac{2\pi ik}{L}(l-n)}\sin^2(\frac{\theta_k}{2})\\ =&\frac{1}{L}\sum_k e^{-\frac{2\pi ik}{L}(l-n)}\frac{1}{2}\Big(1-\cos\theta_k\Big)\end{aligned} \tag{3.14}$$

Since in XX model $\gamma = 0$ then we have $\sin(\theta_k) = 0$. One can write for the expression in parenthesis as:

$$\frac{1}{2}(1-\cos\theta_k) = \frac{\varepsilon_k - J\cos\phi_k + h}{2\varepsilon_k} = \begin{cases}0 & J\cos\phi_k > h\\ 1 & J\cos\phi_k < h\end{cases}.$$

Using this result, we get

$$\left\langle c_l^\dagger c_n\right\rangle = \frac{1}{L}\sum_{k=1}^{L}e^{-\frac{2\pi ik}{L}(l-n)}\Theta\Big(h - J\cos\phi_k\Big) \tag{3.15}$$

where $\Theta(x)$ is the Heaviside step function, meaning $\Theta(x) = 1$ for $x > 0$ and zero otherwise. Therefore, with this set of parameters, we have $k^* = [\frac{L}{2\pi}\cos^{-1}(\frac{h}{J})]$ which corresponds to non-vanishing terms of the sum (we set $n_c = \cos^{-1}(\frac{h}{J})$). Note that here, we will be doing

the calculations for general n_c (consequently h) which the ground state of the system is not degenerate. Therefore, we can rewrite the (3.15) as:

$$\left\langle c_l^\dagger c_n \right\rangle = \frac{1}{L}\sum_{k=1}^{k^*} e^{\frac{2\pi i k}{L}(l-n)} + \frac{1}{L}\sum_{k=L-k^*}^{L} e^{\frac{2\pi i k}{L}(l-n)}$$

With a shift in dummy indices of the second term ($k \to k+L$), this equation can be written as

$$\begin{aligned}\left\langle c_l^\dagger c_n \right\rangle =& \frac{1}{L}\sum_{k=1}^{k^*} e^{\frac{2\pi i k}{L}(l-n)} + \frac{1}{L}\sum_{k=-k^*}^{0} e^{\frac{2\pi i k}{L}(l-n)} = \frac{1}{L} + \frac{2}{L}\sum_{k=1}^{k^*}\cos(\frac{2\pi i k}{L}(l-n)) \\ =& \frac{1}{L} + \frac{1}{L}\frac{\sin(q_F(l-n))}{\sin\frac{\pi}{L}(l-n)} - \frac{1}{L}\end{aligned}$$

where $q_F = n_c + \frac{\pi}{L} = \frac{2\pi}{L}(k^* + \frac{1}{2})$.To calculate above we have used $\sum_{n=0}^{N}\cos n\theta = \frac{1}{2} + \frac{\sin(N+\frac{1}{2})\theta}{2\sin\frac{\theta}{2}}$. Using this result for correlation matrix, one can write:

$$\begin{aligned} C_{ij} =& \frac{1}{L}\frac{\sin(q_F(i-j))}{\sin\frac{\pi}{L}(i-j)}; \qquad i \neq j, \\ C_{ii} =& \frac{n_c}{\pi} + \frac{1}{L}. \end{aligned} \tag{3.16}$$

which is the analytic expression for the correlation matrix of XX model in the ground state with periodic boundary conditions. To find the correlation matrix of an infinite chain in its ground state we just use the result of (3.16) with $L \to \infty$. In particular, in this limit we have $q_F \sim n_c$ and $\sin\frac{\pi}{L}(i-j) \sim \frac{\pi}{L}(i-j)$. Elemnts of $\mathbf{C}$ simplifies to:

$$\begin{aligned} C_{ij} =& \frac{\sin(n_c(i-j))}{\pi(i-j)}; \qquad i \neq j \\ C_{ii} =& \frac{n_c}{\pi} \end{aligned} \tag{3.17}$$

In the OBC, it is also easy to do same calculations for XX case, details of the calculation are not presented here. Using the results of section 2.4.2, I can write:

$$\left\langle \eta_k^\dagger \eta_q \right\rangle = \delta_{k,q}\Theta\Big(h - J\cos(\frac{\pi k}{L+1})\Big).$$

The fermionic two-point correlation $\mathbf{C}$ can be obtained by

$$C_{mn} = \frac{1}{2(L+1)}\left[\frac{\sin(q_F(n-m))}{\sin(\alpha(n-m))} - \frac{\sin(q_F(n+m))}{\sin(\alpha(n+m))}\right]; \qquad n \neq m. \tag{3.18}$$

Where $\alpha = \frac{\pi}{2(L+1)}$ and $q_F = n_c + \alpha$ and $n_c = \cos^{-1}(\frac{h}{J})$. For the diagonal elements $n = m$, we have

$$C_{nn} = \frac{n_c}{\pi} + \frac{1}{2(L+1)} - \frac{1}{L+1}\frac{\sin(2q_F n)}{\sin(2\alpha n)} = \frac{n_c}{\pi} + \begin{cases} 0 & n \text{ even} \\ \frac{1}{L+1} & n \text{ odd} \end{cases}. \tag{3.19}$$

Finally, a semi-finite system is the open chain with the limit $L \to \infty$ and its correlations are given by:

$$\begin{aligned} C_{nn} =& \frac{n_c}{\pi} \\ C_{nm} =& \frac{\sin n_c(n-m)}{\pi(n-m)} - \frac{\sin n_c(n+m)}{\pi(n+m)}. \end{aligned} \tag{3.20}$$

3.1.2 Correlations for excited eigenstates

In this section, we want to calculate the correlation matrices for excited eigenstates of Hamiltonian as introduced in 2.3.4. The formulas in 3.1.1 can be also generalized to the excited states. The generic excited state is defined as:

$$|\psi\rangle = |k_1, ..., k_j\rangle = \eta^\dagger_{k_1} ... \eta^\dagger_{k_j} |0\rangle \,, \tag{3.21}$$

Having η-operators allows us to write the correlation matrix of interest in terms of $\mathbf{U}$ (and $\mathbf{U}^\dagger$). For instance.

$$\langle c^\dagger_i c_j \rangle_\psi = \langle 0| \prod_{k_j \in \mathbb{E}} \eta_{k_j} \sum_{k,l} (h^*_{li} \eta_l + g_{ki} \eta^\dagger_k) \sum_{n,m} (g^*_{mj} \eta_m + h_{nj} \eta^\dagger_n) \prod_{k_j \in \mathbb{E}} \eta^\dagger_{k_j} |0\rangle \,, \tag{3.22}$$

$$\langle c^\dagger_i c^\dagger_j \rangle_\psi = \langle 0| \prod_{k_j \in \mathbb{E}} \eta_{k_j} \sum_{k,l} (h^*_{li} \eta_l + g_{ki} \eta^\dagger_k) \sum_{n,m} (h^*_{mj} \eta_m + g_{nj} \eta^\dagger_n) \prod_{k_j \in \mathbb{E}} \eta^\dagger_{k_j} |0\rangle \,. \tag{3.23}$$

Using the Wick theorem we can simplify these expression to get:

$$\begin{aligned} \langle c^\dagger_i c_j \rangle_\psi &= (\mathbf{h}^\dagger . \mathbf{h})_{i,j} + \sum_{k_j \in \mathbb{E}} (g_{k_j,i} g^*_{k_j,j} - h^*_{k_j,i} h_{k_j,j}), \\ \langle c^\dagger_i c^\dagger_j \rangle_\psi &= (\mathbf{h}^\dagger . \mathbf{g})_{i,j} + \sum_{k_j \in \mathbb{E}} (g_{k_j,i} h^*_{k_j,j} - h^*_{k_j,i} g_{k_j,j}). \end{aligned} \tag{3.24}$$

Therefore, using the definitions (3.4), we get

$$\begin{aligned} \mathbf{K}^\psi_{ij} =& (\mathbf{h}^\dagger + \mathbf{g}^\dagger).(\mathbf{h} + \mathbf{g})_{ij} + \sum_{k_j \in \mathbb{E}} g_{k_j,i} g^*_{k_j,j} + \sum_{k_j \in \mathbb{E}} g_{k_j,i} h^*_{k_j,j} - \sum_{k_j \in \mathbb{E}} h^*_{k_j,i} g_{k_j,j} - \sum_{k_j \in \mathbb{E}} h^*_{k_j,i} h_{k_j,j} \\ & - \sum_{k_j \in \mathbb{E}} g^*_{k_j,i} g_{k_j,j} - \sum_{k_j \in \mathbb{E}} g^*_{k_j,i} h_{k_j,j} + \sum_{k_j \in \mathbb{E}} h_{k_j,i} g^*_{k_j,j} + \sum_{k_j \in \mathbb{E}} h_{k_j,i} h^*_{k_j,j} \\ =& (\mathbf{h}^\dagger + \mathbf{g}^\dagger).(\mathbf{h} + \mathbf{g})_{ij} - \sum_{k_j \in \mathbb{E}} (h^*_{k_j,i} + g^*_{k_j,i})(g_{k_j,j} + h_{k_j,j}) + \sum_{k_j \in \mathbb{E}} (h_{k_j,i} + g_{k_j,i})(g^*_{k_j,j} + h^*_{k_j,j}), \end{aligned}$$

$$\begin{aligned} \bar{\mathbf{K}}^\psi_{ij} =& (\mathbf{h}^\dagger - \mathbf{g}^\dagger).(\mathbf{h} - \mathbf{g})_{ij} + \sum_{k_j \in \mathbb{E}} g_{k_j,i} g^*_{k_j,j} - \sum_{k_j \in \mathbb{E}} g_{k_j,i} h^*_{k_j,j} + \sum_{k_j \in \mathbb{J}} h^*_{k_j,i} g_{k_j,j} - \sum_{k_j \in \mathbb{E}} h^*_{k_j,i} h_{k_j,j} \\ & - \sum_{k_j \in \mathbb{E}} g^*_{k_j,i} g_{k_j,j} + \sum_{k_j \in \mathbb{E}} g^*_{k_j,i} h_{k_j,j} - \sum_{k_j \in \mathbb{E}} h_{k_j,i} g^*_{k_j,j} + \sum_{k_j \in \mathbb{E}} h_{k_j,i} h^*_{k_j,j} \\ =& (\mathbf{h}^\dagger - \mathbf{g}^\dagger).(\mathbf{h} - \mathbf{g})_{ij} - \sum_{k_j \in \mathbb{E}} (h^*_{k_j,i} - g^*_{k_j,i})(h_{k_j,j} - g_{k_j,j}) + \sum_{k_j \in \mathbb{E}} (h_{k_j,i} - g_{k_j,i})(h^*_{k_j,j} - g^*_{k_j,j}), \end{aligned}$$

$$\begin{aligned} \mathbf{G}^\psi_{ij} =& (\mathbf{h}^\dagger - \mathbf{g}^\dagger).(\mathbf{h} + \mathbf{g})_{ij} + \sum_{k_j \in \mathbb{E}} g_{k_j,i} g^*_{k_j,j} + \sum_{k_j \in \mathbb{E}} g_{k_j,i} h^*_{k_j,j} - \sum_{k_j \in \mathbb{E}} h^*_{k_j,i} g_{k_j,j} - \sum_{k_j \in \mathbb{E}} h^*_{k_j,i} h_{k_j,j} \\ & + \sum_{k_j \in \mathbb{E}} g^*_{k_j,i} g_{k_j,j} + \sum_{k_j \in \mathbb{E}} g^*_{k_j,i} h_{k_j,j} - \sum_{k_j \in \mathbb{E}} h_{k_j,i} g^*_{k_j,j} - \sum_{k_j \in \mathbb{E}} h_{k_j,i} h^*_{k_j,j} \\ =& (\mathbf{h}^\dagger - \mathbf{g}^\dagger).(\mathbf{h} + \mathbf{g})_{ij} + \sum_{k_j \in \mathbb{E}} (g^*_{k_j,i} - h^*_{k_j,i})(h_{k_j,j} + g_{k_j,j}) + \sum_{k_j \in \mathbb{E}} (g_{k_j,i} - h_{k_j,i})(h^*_{k_j,j} + g^*_{k_j,j}). \end{aligned}$$

We can write them in a shorter version

$$\mathbf{K}^\psi_{ij} = (\mathbf{h}^\dagger + \mathbf{g}^\dagger).(\mathbf{h} + \mathbf{g})_{ij} - 2i\Im\Big[\sum_{k_j \in \mathbb{E}} (h^*_{k_j,i} + g^*_{k_j,i})(g_{k_j,j} + h_{k_j,j}) \Big], \tag{3.25}$$

$$\bar{\mathbf{K}}^{\psi}_{ij} =(\mathbf{h}^{\dagger} - \mathbf{g}^{\dagger}).(\mathbf{h} - \mathbf{g})_{ij} - 2i\Im\Big[\sum_{k_j\in\mathbb{E}}(h^{*}_{k_j,i} - g^{*}_{k_j,i})(h_{k_j,j} - g_{k_j,j})\Big], \tag{3.26}$$

$$\mathbf{G}^{\psi}_{ij} =(\mathbf{h}^{\dagger} - \mathbf{g}^{\dagger}).(\mathbf{h} + \mathbf{g})_{ij} + 2\Re\Big[\sum_{k_j\in\mathbb{E}}(g^{*}_{k_j,i} - h^{*}_{k_j,i})(h_{k_j,j} + g_{k_j,j})\Big]. \tag{3.27}$$

Then after some algebra one can show that

$$\mathbf{C}_{\{k_1,...,k_l\}} = \mathbf{h}^{\dagger}.\mathbf{h} + \mathbf{g}^{T}.\mathbf{I}'.\mathbf{g}^{*} - \mathbf{g}^{\dagger}.\mathbf{I}'.\mathbf{h}, \tag{3.28}$$

$$\mathbf{F}_{\{k_1,...,k_l\}} = \mathbf{h}^{\dagger}.\mathbf{g} + \mathbf{g}^{T}.\mathbf{I}'.\mathbf{h}^{*} - \mathbf{h}^{\dagger}.\mathbf{I}'.\mathbf{g}, \tag{3.29}$$

where

$$I'_{kk'} = \begin{cases} \delta_{kk'} & : k \in \{k_1, ..., k_l\} \\ 0 & : \text{otherwise} \end{cases} \tag{3.30}$$

Then one can also show that

$$\mathbf{G}_{\{k_1,...,k_l\}} = (\mathbf{h}^{\dagger} - \mathbf{g}^{\dagger})(\mathbf{h} + \mathbf{g}) - 2\mathrm{Re}[(\mathbf{h}^{\dagger} - \mathbf{g}^{\dagger}).\mathbf{I}'.(\mathbf{h} + \mathbf{g})], \tag{3.31}$$

$$\mathbf{K}_{\{k_1,...,k_l\}} = (\mathbf{h}^{\dagger} + \mathbf{g}^{\dagger})(\mathbf{h} + \mathbf{g}) - 2i\mathrm{Im}[(\mathbf{h}^{\dagger} + \mathbf{g}^{\dagger}).\mathbf{I}'.(\mathbf{h} + \mathbf{g})], \tag{3.32}$$

$$\bar{\mathbf{K}}_{\{k_1,...,k_l\}} = (\mathbf{h}^{\dagger} - \mathbf{g}^{\dagger})(\mathbf{h} - \mathbf{g}) - 2i\mathrm{Im}[(\mathbf{h}^{\dagger} - \mathbf{g}^{\dagger}).\mathbf{I}'.(\mathbf{h} - \mathbf{g})]. \tag{3.33}$$

As an example, if all the modes are excited then the state would be $|\phi\rangle = \prod_{\text{all } k_j} \eta^{\dagger}_{k_j} |0\rangle$. Therefore for the correlation matrices we would get

$$\mathbf{K}^{\phi} = \Big(\mathbf{h}^{T} + \mathbf{g}^{T}\Big).\Big(\mathbf{h}^{*} + \mathbf{g}^{*}\Big) = 2 \times \mathbb{1} - \Big(\mathbf{h}^{\dagger} + \mathbf{g}^{\dagger}\Big).\Big(\mathbf{h} + \mathbf{g}\Big) = 2 \times \mathbb{1} - \mathbf{K}^{0}, \tag{3.34}$$

$$\bar{\mathbf{K}}^{\phi} = \Big(\mathbf{h}^{T} - \mathbf{g}^{T}\Big).\Big(\mathbf{h}^{*} - \mathbf{g}^{*}\Big) = 2 \times \mathbb{1} - \Big(\mathbf{h}^{\dagger} - \mathbf{g}^{\dagger}\Big).\Big(\mathbf{h} - \mathbf{g}\Big) = 2 \times \mathbb{1} - \bar{\mathbf{K}}^{0}, \tag{3.35}$$

and

$$\mathbf{G}^{\phi} = \Big(\mathbf{g}^{T} - \mathbf{h}^{T}\Big).\Big(\mathbf{h}^{*} + \mathbf{g}^{*}\Big) = \Big(\mathbf{g}^{\dagger} - \mathbf{h}^{\dagger}\Big).\Big(\mathbf{h} + \mathbf{g}\Big) = -\mathbf{G}^{0}. \tag{3.36}$$

Looking at these expressions, there is an interesting similarity between these correlations and those of ground state. First, we know that in all the quadratic fermionic models, the spectrum is symmetric. Therefore, the energy of highly excited eigenstate would be the opposite sign of the ground state energy. This can be achieved by changing η to $\eta^{\dagger}$. Or, we can change $\mathbf{A}$ to $-\mathbf{A}$ and $\mathbf{B}$ to $-\mathbf{B}$. Now, to keep the convention the same (after the diagonalizatio, first comes the positive eigenvalues and then the negative ones), we would need to put $\mathbf{g} \to \mathbf{h}^{*}$ and $\mathbf{h} \to \mathbf{g}^{*}$ in the unitary matrix (2.49) which diagolize the Hamiltonian. This new unitary matrix $\mathbf{U}'$ has the relation:

$$\mathbf{U}' = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ \mathbf{1} & \mathbf{0} \end{pmatrix} . \begin{pmatrix} \mathbf{g} & \mathbf{h} \\ \mathbf{h}^{*} & \mathbf{g}^{*} \end{pmatrix} . \tag{3.37}$$

With this transformation, we can see the relation between correlation matrices (3.34-3.36). Another argument could be the relation between **C** and **F** matrix for vacuum and highly excited eigenstate. For instance, $\eta_j^\dagger |\phi\rangle = 0$, for all j's then

$$\langle c_i^\dagger c_j\rangle_\phi = \langle\phi| \left(h_{li}^* \eta_l + g_{ki}\eta_k^\dagger\right)\left(g_{mj}^*\eta_m + h_{nj}\eta_n^\dagger\right)|\phi\rangle = \langle\phi| g_{ki}\eta_k^\dagger g_{mj}^*\eta_m |\phi\rangle = g_{mi}g_{mj}^*.$$

Therefore, it can be verified that

$$\mathbf{C}^\phi = \mathbf{1} - \mathbf{C}^0, \quad \text{and} \quad \mathbf{F}^\phi = -\mathbf{F}^0.$$

When substitute in (3.4), then we would reach the expression (3.34)-(3.36).

The above observation is called *Particle-Hole Duality* and it suggest the following relations between the matrices corresponding to the excited state $\{k_1, ..., k_l\}$ and the one with the complement modes excited, i.e. $\{k_{l+1}, ..., k_N\}$:

$$\mathbf{G}_{\{k_1,...,k_l\}} + \mathbf{G}_{\{k_{l+1},...,k_N\}} = 0 \tag{3.38}$$

$$\mathbf{K}_{\{k_1,...,k_l\}} + \mathbf{K}_{\{k_{l+1},...,k_N\}} = 2\mathbf{I} \tag{3.39}$$

$$\bar{\mathbf{K}}_{\{k_1,...,k_l\}} + \bar{\mathbf{K}}_{\{k_{l+1},...,k_N\}} = 2\mathbf{I}. \tag{3.40}$$

The above relations suggest similar physics for the two complement excited states or equivalently, particles and holes.

3.1.3 Relation of $\mathbf{R}$ matrix and correlation matrices

The matrix **R** can be written in terms of correlation matrices of section 3.1 [13, 14]. For instant, in the simple case where entries of **A** and **B** are real in Hamiltonian (2.35), we have $\mathbf{R} = \frac{\mathbb{I}+\mathbf{G}}{\mathbb{I}-\mathbf{G}}$ where **G** being the correlation matrix with the elements $G_{ij} = \langle(c_i^\dagger - c_i)(c_i^\dagger + c_i)\rangle$ as define in (3.3). To prove the latter, we use the results of (3.9):

$$\begin{aligned}
\mathbb{I} + \mathbf{G} =& (\mathbf{h}^T - \mathbf{g}^T)(\mathbf{h} + \mathbf{g}) + \mathbb{I} = -\mathbf{g}^T\mathbf{h} - \mathbf{g}^T\mathbf{g} + \mathbf{h}^T\mathbf{h} + \mathbf{h}^T\mathbf{g} + \mathbb{I} \\
=& 2(\mathbf{h}^T - \mathbf{g}^T)\mathbf{h} \\
\mathbb{I} - \mathbf{G} =& \mathbb{I} - (\mathbf{g}^T - \mathbf{h}^T)(\mathbf{h} + \mathbf{g}) = \mathbf{g}^T\mathbf{h} + \mathbf{g}^T\mathbf{g} - \mathbf{h}^T\mathbf{h} - \mathbf{h}^T\mathbf{g} + \mathbb{I} \\
=& -2(\mathbf{h}^T - \mathbf{g}^T)\mathbf{g}
\end{aligned}$$

Therefore,

$$\frac{\mathbb{I} + \mathbf{G}}{\mathbb{I} - \mathbf{G}} = (\mathbb{I} - \mathbf{G})^{-1}(\mathbb{I} + \mathbf{G}) = -\mathbf{g}^{-1}\mathbf{h} = \mathbf{R}. \tag{3.41}$$

In a general case where **g** and **h** are matrices with complex entries then we have a complicated relation between correlations and **R** matrix. For instance we start by calculate the elements of **G** (3.3) for the state (2.53).

$$G_{ij} = \langle 0|\,(c_i^\dagger - c_i)(c_j^\dagger + c_j)\,|0\rangle = \langle c_i^\dagger c_j\rangle + \langle c_i^\dagger c_j^\dagger\rangle - \langle c_i c_j\rangle - \langle c_i c_j^\dagger\rangle \tag{3.42}$$

To calculate each of the expectation values above, first we use the Fermionic coherent state defined as

$$|\boldsymbol{\xi}\rangle = |\xi_1\xi_2\cdots\xi_N\rangle = e^{-\sum_{k=1}^{N}\xi_k c_k^\dagger}\,|0\rangle_c\,, \tag{3.43}$$

where ξ_k are Grassmann variables. For more details on fermion coherent state see Appendix A and [13, 58]. To proceed, we can use the Identity resolution of Grassmann variables

$$\mathbf{I} = \int \prod_l \mathrm{d}\bar{\xi}_l \mathrm{d}\xi_l e^{-\bar{\boldsymbol{\xi}}\cdot\boldsymbol{\xi}}\,|\boldsymbol{\xi}\rangle\langle\boldsymbol{\xi}| \tag{3.44}$$

Then, we use (3.43), and reorder each term by moving every c operator to the left.

$$\langle c_i c_j\rangle = |C|^2{}_c\langle 0|\, e^{-\frac{1}{2}R^*_{mn}c_m c_n} c_i c_j e^{\frac{1}{2}R_{lk}c_l^\dagger c_k^\dagger}\,|0\rangle_c = |C|^2 \int \prod \mathrm{d}\bar{\xi}_{l'}\mathrm{d}\xi_{l'}\xi_i\xi_j e^{-\bar{\xi}_r\xi_r} e^{\frac{1}{2}R_{lk}\bar{\xi}_l\bar{\xi}_k - \frac{1}{2}R^*_{mn}\xi_m\xi_n},$$

$$\langle c_i^\dagger c_j\rangle = |C|^2{}_c\langle 0|\, e^{-\frac{1}{2}R^*_{mn}c_m c_n} c_i^\dagger c_j e^{\frac{1}{2}R_{lk}c_l^\dagger c_k^\dagger}\,|0\rangle_c = \delta_{ij} - |C|^2 \int \prod \mathrm{d}\bar{\xi}_{l'}\mathrm{d}\xi_{l'}\xi_j\bar{\xi}_i e^{-\bar{\xi}_r\xi_r} e^{\frac{1}{2}R_{lk}\bar{\xi}_l\bar{\xi}_k - \frac{1}{2}R^*_{mn}\xi_m\xi_n},$$

$$\langle c_i c_j^\dagger\rangle = |C|^2{}_c\langle 0|\, e^{-\frac{1}{2}R^*_{mn}c_m c_n} (\delta_{ij} - c_j^\dagger c_i) e^{\frac{1}{2}R_{lk}c_l^\dagger c_k^\dagger}\,|0\rangle_c = |C|^2 \int \prod \mathrm{d}\bar{\xi}_{l'}\mathrm{d}\xi_{l'}\xi_i\bar{\xi}_j e^{-\bar{\xi}_r\xi_r} e^{\frac{1}{2}R_{lk}\bar{\xi}_l\bar{\xi}_k - \frac{1}{2}R^*_{mn}\xi_m\xi_n},$$

$$\langle c_i^\dagger c_j^\dagger\rangle = |C|^2{}_c\langle 0|\, e^{-\frac{1}{2}R^*_{mn}c_m c_n} c_i^\dagger c_j^\dagger e^{\frac{1}{2}R_{lk}c_l^\dagger c_k^\dagger}\,|0\rangle_c = |C|^2 \int \prod \mathrm{d}\bar{\xi}_{l'}\mathrm{d}\xi_{l'}\bar{\xi}_i\bar{\xi}_j e^{-\bar{\xi}_r\xi_r} e^{\frac{1}{2}R_{lk}\bar{\xi}_l\bar{\xi}_k - \frac{1}{2}R^*_{mn}\xi_m\xi_n},$$

With this method, we need to solve the Grassmann integration containing combination of ξ and $\bar{\xi}$. To solve the integrals above, we introduce a new Grassmann variable $\boldsymbol{\eta}^T = \begin{pmatrix}\bar{\boldsymbol{\xi}} & \boldsymbol{\xi}\end{pmatrix}$. Then we can write the integral as. $\langle\cdots\rangle = |C|^2 \int \mathbf{D}\boldsymbol{\eta}\,(\eta_{J_1}\eta_{J_2}) e^{\frac{1}{2}\boldsymbol{\eta}^T\mathbf{A}\boldsymbol{\eta}}$ with $\mathbf{A} = \begin{pmatrix}\mathbf{R} & -\mathbf{I}\\ \mathbf{I} & -\mathbf{R}^*\end{pmatrix}$.

Using equation (A.8), we get $\mathrm{Pf}[\mathbf{A}] = \sqrt{\det[\mathbb{I} + \mathbf{R}^\dagger\mathbf{R}]}$ and

$$\mathbf{A}^{-T} = \begin{bmatrix} -\mathbf{R}^{-1} - \mathbf{R}^{-1}(\mathbf{R}^* - \mathbf{R}^{-1})^{-1}\mathbf{R}^{-1} & (\mathbf{R}^* - \mathbf{R}^{-1})^{-1}\mathbf{R}^{-1} \\ -\mathbf{R}^{-1}(\mathbf{R}^* - \mathbf{R}^{-1})^{-1} & (\mathbf{R}^* - \mathbf{R}^{-1})^{-1} \end{bmatrix} = \begin{bmatrix} \mathbf{R}^*(\mathbf{I} - \mathbf{R}^*\mathbf{R})^{-1} & -(\mathbf{I} - \mathbf{R}^*\mathbf{R})^{-1} \\ (\mathbf{I} - \mathbf{R}\mathbf{R}^*)^{-1} & (\mathbf{I} - \mathbf{R}^*\mathbf{R})^{-1}\mathbf{R} \end{bmatrix} \tag{3.45}$$

In our case, the set J as introduced in (A.8), Appendix A, contains only two indexes ($J = \{J_1, J_2\}$), therefore $\mathrm{Pf}\left[(\mathbf{A}^{-T})_{JJ}\right] = (\mathbf{A}^{-T})_{J_1J_2}$. This means we can look for the solution each expectation value in the submatrices of $\mathbf{A}^{-T}$. To reduce the calculations we just calculate the correlation matrices $\mathbf{C} = \langle c_i^\dagger c_j\rangle$ and $\mathbf{F} = \langle c_i^\dagger c_j^\dagger\rangle$

$$\mathbf{C} = \mathbf{I} - \mathbf{Q}, \qquad \mathbf{F} = \mathbf{R}^*\mathbf{Q}^T \qquad \text{where} \quad \mathbf{Q} = (\mathbf{I} - \mathbf{R}^*\mathbf{R})^{-1} \tag{3.46}$$

Using this result and equation (3.4), we get:

$$\begin{aligned} \mathbf{G} &= \mathbf{I} + \mathbf{Q}(\mathbf{R}^* - \mathbf{I}) + (\mathbf{R} - \mathbf{I})\mathbf{Q}^T, \\ \mathbf{K} &= (\frac{1}{2}\mathbf{I} + \mathbf{R}^*)\mathbf{Q}^T + \mathbf{Q}^T(\frac{1}{2}\mathbf{I} - \mathbf{R}) - \mathbf{Q} + \mathbf{I} \\ \bar{\mathbf{K}} &= (\frac{1}{2}\mathbf{I} - \mathbf{R}^*)\mathbf{Q}^T + \mathbf{Q}^T(\frac{1}{2}\mathbf{I} + \mathbf{R}) - \mathbf{Q} + \mathbf{I} \end{aligned} \tag{3.47}$$

Since we are interested in a relation to write the vacuum in exponential form (2.53). Then it is useful to mention $\mathbf{R} = \mathbf{F}^*(\mathbf{I} - \mathbf{C})^{-1}$. The result above for the case where $\mathbf{R}$ is a real matrix, we get equation (3.41).

It can also be concluded that the same relation is valid among the correlation matrices and $\mathbf{R}$ matrix for an excited eigenstate (see sections 2.3.4 and 3.1.2).

$$\begin{aligned}
\mathbf{G}^{\psi} &= \mathbf{I} + \mathbf{Q}^{\psi}(\mathbf{R}^{\psi^*} - \mathbf{I}) + (\mathbf{R}^{\psi} - \mathbf{I})\mathbf{Q}^{\psi^T}, \\
\mathbf{K}^{\psi} &= (\frac{1}{2}\mathbf{I} + \mathbf{R}^{\psi^*})\mathbf{Q}^{\psi^T} + \mathbf{Q}^{\psi^T}(\frac{1}{2}\mathbf{I} - \mathbf{R}^{\psi}) - \mathbf{Q}^{\psi} + \mathbf{I} \\
\bar{\mathbf{K}}^{\psi} &= (\frac{1}{2}\mathbf{I} - \mathbf{R}^{\psi^*})\mathbf{Q}^{\psi^T} + \mathbf{Q}^{\psi^T}(\frac{1}{2}\mathbf{I} + \mathbf{R}^{\psi}) - \mathbf{Q}^{\psi} + \mathbf{I}
\end{aligned} \tag{3.48}$$

where $\mathbf{Q}^{\psi} = (\mathbf{I} - \mathbf{R}^{\psi^*}\mathbf{R}^{\psi})^{-1}$ and $\mathbf{R}^{\psi}$ is defined in (2.64).

— 4 —

Density matrix formulation

4.1 Density matrix formulation

A density matrix is a matrix that describes the statistical state of a system in quantum mechanics. The probability for any outcome of any well-defined measurement upon a system can be calculated from the density matrix for that system. The Entanglement entropy of a state can be expressed in terms of the eigenvalues of density matrix.

In this part, we use the Grassmann variables to write the coherent state for fermions. Then, we can drive the expression of the reduced density matrix (RDM) and entanglement entropy for the desired states using the Grassmann integrals (see Appendix A). A coherent state for fermions is defined as

$$|\boldsymbol{\xi}\rangle = |\xi_1 \xi_2 \cdots \xi_N\rangle = e^{-\sum_{k=1}^{N} \xi_k c_k^\dagger} |0\rangle_c \,, \tag{4.1}$$

where $|0\rangle_c$ is annihilated by all the c_k operators. One can verify that

$$c_i |\boldsymbol{\xi}\rangle = \xi_i |\boldsymbol{\xi}\rangle \,, \quad \langle\boldsymbol{\xi}| c_i^\dagger = \langle\boldsymbol{\xi}| \bar{\xi}_i, \quad {}_c\langle 0|\boldsymbol{\xi}\rangle = 1. \tag{4.2}$$

4.1.1 Density matrix for vacuum state

Using the above expressions and (2.53), we start by writing the density matrix for the vacuum state

$$\rho = |C|^2 e^{\frac{1}{2}\sum_{i,j} R_{ij} c_i^\dagger c_j^\dagger} |0\rangle_c \, {}_c\langle 0| \, e^{\frac{1}{2}\sum_{i,j} -R_{ij}^* c_i c_j}, \tag{4.3}$$

and $C = \frac{1}{\sqrt[4]{\det[\mathbf{I}+\mathbf{R}^\dagger\mathbf{R}]}}$. Now we write the matrix form of density operator in terms of Grassmann variables using (A.16).

$$\rho(\boldsymbol{\xi}, \boldsymbol{\xi}') = \langle\boldsymbol{\xi}| \rho |\boldsymbol{\xi}'\rangle = |C|^2 \, e^{\frac{1}{2}\sum_{i,j} R_{ij} \bar{\xi}_i \bar{\xi}_j} \, e^{-\frac{1}{2}\sum_{i,j} R_{ij}^* \xi_i' \xi_j'}. \tag{4.4}$$

To calculate the reduced density matrix, we divide the system into two parts (sets) $\mathbb{1}$ and $\mathbb{2}$ where the full system is given by $\mathbb{1} + \mathbb{2}$. we trace out fermions in the subsystem $\mathbb{2}$ to find the RDM for subsystem $\mathbb{1}$, $\rho_{\mathbb{1}} = \mathrm{tr}_{\mathbb{2}} \rho$. In other words, we are calculating the entanglement of the fermions of subsystem D with the rest of the system. To trace out the unwanted parts, we use equation (D.54b).

$$\rho_{\mathbb{1}}(\boldsymbol{\xi}, \boldsymbol{\xi}') = \int \prod_{l\in\mathbb{2}} \mathrm{d}\bar{\xi}_l \mathrm{d}\xi_l \; e^{-\sum_{n\in\mathbb{2}} \bar{\xi}_n \xi_n} \, \langle \xi_1, \cdots, \xi_k, -\xi_{k+1}, \cdots, -\xi_L| \, \rho \, |\xi_1', \cdots, \xi_k', \xi_{k+1}, \cdots, \xi_L\rangle \,, \tag{4.5}$$

where indexes $\{1, \cdots, k\} \in \mathbb{1}$ and $\{k+1, \cdots, L\} \in \mathbb{2}$. Since all the terms in the expression above are quadratic in Grassmann variables, we can write them in the same argument[1]. Also, we can move out those variables that are not in the integral. Therefore, we are left with

$$\begin{aligned} \rho_{\mathbb{1}}(\boldsymbol{\xi}, \boldsymbol{\xi}') = & |C|^2 e^{\frac{1}{2}(\mathbf{R}_{11})_{ij}\bar{\xi}_i\bar{\xi}_j - \frac{1}{2}(\mathbf{R}_{11}^*)_{ji}\xi_j'\xi_i'} \int \prod_{l\in\mathbb{2}} \mathrm{d}\bar{\xi}_l \mathrm{d}\xi_l \; e^{-\bar{\xi}_n\xi_n} \Big[e^{-\frac{1}{2}(\mathbf{R}_{12})_{in}\bar{\xi}_i\bar{\xi}_n - \frac{1}{2}(\mathbf{R}_{21})_{ni}\bar{\xi}_n\bar{\xi}_i} \\ & \times e^{\frac{1}{2}(\mathbf{R}_{22})_{mn}\bar{\xi}_m\bar{\xi}_n} e^{-\frac{1}{2}(\mathbf{R}_{22}^*)_{nm}\xi_n\xi_m + \frac{1}{2}(\mathbf{R}_{12}^*)_{jm}\xi_j'\xi_m + \frac{1}{2}(\mathbf{R}_{21}^*)_{mj}\xi_m\xi_j'} \Big] \end{aligned} \tag{4.6}$$

[1] $e^{\mathbf{A}} e^{\mathbf{B}} = e^{\mathbf{A}+\mathbf{B}}$

where in the above Einstein summation convention is used, and indexes $i, j \in \mathbb{1}$ where indexes $n, m \in \mathbb{2}$. Equivalently, we divides $\mathbf{R}$ into four submatrices $\mathbf{R_{11}}$, $\mathbf{R_{12}}$, $\mathbf{R_{21}} = -\mathbf{R_{12}}^T$ and $\mathbf{R_{22}}$, according to whether the sites i,j,n,m belong to the part we are tracing out or not. Although these submatrices do not need to have the same size, $\mathbf{R_{11}}$ and $\mathbf{R_{22}}$ are square matrices. Those parts that are at the back of integral we denote by $\mathcal{F}(\{\xi_i'\}, \{\bar{\xi}_j\})$. Going back to the reduced density matrix, we can rewrite it in the Gaussian form of

$$\rho_{\mathbb{1}}(\boldsymbol{\xi}, \boldsymbol{\xi}') = \mathcal{F}(\{\xi_i'\}, \{\bar{\xi}_j\}) \int \prod_{l \in \mathbb{2}} \mathrm{d}\bar{\xi}_l \mathrm{d}\xi_l \, e^{\frac{1}{2}\begin{pmatrix}\bar{\xi} & \xi\end{pmatrix}\boldsymbol{\mathcal{A}}\begin{pmatrix}\bar{\xi} \\ \xi\end{pmatrix} + \boldsymbol{\zeta}\boldsymbol{\xi} + \boldsymbol{\kappa}\bar{\boldsymbol{\xi}}}. \tag{4.7}$$

where matrix $\boldsymbol{\mathcal{A}}$ can be thought of as a block matrix

$$\boldsymbol{\mathcal{A}} = \begin{pmatrix} \mathbf{R}_{22} & -\mathbf{I} \\ \mathbf{I} & -\mathbf{R}_{22}^* \end{pmatrix}$$

In addition $\boldsymbol{\zeta} = -\boldsymbol{\xi}'\mathbf{R}_{12}{}^*$ and $\boldsymbol{\kappa} = -\bar{\boldsymbol{\xi}}\mathbf{R}_{12}$. Now to calculate the partial trace we have to define new Grassmann variables

Now, for reduced density matrix we have:

$$\rho_{\mathbb{1}}(\boldsymbol{\xi}, \boldsymbol{\xi}') = \mathcal{F}(\{\xi_i'\}, \{\bar{\xi}_j\}) \int \mathbf{D}\boldsymbol{\eta} \, e^{\frac{1}{2}\eta^T \boldsymbol{\mathcal{A}} \eta + \lambda^T \eta}. \tag{4.8}$$

Using the equation (A.7), we can solve the integral. After the integration we have:

$$\rho_{\mathbb{1}}(\boldsymbol{\xi}, \boldsymbol{\xi}') = \mathcal{F}(\{\xi_i'\}, \{\bar{\xi}_j\}) \, \mathrm{pf}[\boldsymbol{\mathcal{A}}] e^{\frac{1}{2}\boldsymbol{\lambda}^T \boldsymbol{\mathcal{A}}^{-1} \boldsymbol{\lambda}}. \tag{4.9}$$

Based on formulas for block matrices we have:

$$\boldsymbol{\mathcal{A}}^{-1} = \begin{pmatrix} -(\mathbf{I} - \mathbf{R}_{22}\mathbf{R}_{22}^*)^{-1}\mathbf{R}_{22}\mathbf{R}_{22}^*\mathbf{R}_{22}^{-1} & \left(\mathbf{I} - \mathbf{R}_{22}\mathbf{R}_{22}^*\right)^{-1} \\ -\left(\mathbf{I} - \mathbf{R}_{22}^*\mathbf{R}_{22}\right)^{-1} & (\mathbf{I} - \mathbf{R}_{22}^*\mathbf{R}_{22})^{-1}\mathbf{R}_{22} \end{pmatrix}.$$

Putting it all together, we get for the reduced density matrix

$$\rho_{\mathbb{1}}(\boldsymbol{\xi}, \boldsymbol{\xi}') = \frac{\sqrt{\det[\mathbf{I} + \mathbf{R}_{22}^\dagger \mathbf{R}_{22}]}}{\sqrt{\det[\mathbf{I} + \mathbf{R}^\dagger \mathbf{R}]}} e^{\frac{1}{2}\begin{pmatrix}\bar{\xi} & \xi'\end{pmatrix}\boldsymbol{\Omega}\begin{pmatrix}\bar{\xi} \\ \xi'\end{pmatrix}} \tag{4.10}$$

where $\boldsymbol{\Omega}$ matrix is given by

$$\boldsymbol{\Omega} = \begin{pmatrix} \mathbf{R}_{11} & 0 \\ 0 & -\mathbf{R}_{11}^* \end{pmatrix} + \begin{pmatrix} \mathbf{R}_{12} & 0 \\ 0 & \mathbf{R}_{12}^* \end{pmatrix} \boldsymbol{\mathcal{A}}^{-1} \begin{pmatrix} \mathbf{R}_{12}^T & 0 \\ 0 & \mathbf{R}_{12}^\dagger \end{pmatrix} \tag{4.11}$$

or equivalently

$$\boldsymbol{\Omega} = \begin{pmatrix} \mathbf{R}_{11} + \mathbf{R}_{12}\left[\mathbf{R}_{22} - (\mathbf{R}_{22}^*)^{-1}\right]^{-1}\mathbf{R}_{12}^T & -\mathbf{R}_{12}\mathbf{R}_{22}^{-1}\left(\mathbf{R}_{22}^{-1} - \mathbf{R}_{22}^*\right)^{-1}\mathbf{R}_{12}^\dagger \\ \mathbf{R}_{12}^*\left(\mathbf{R}_{22}^{-1} - \mathbf{R}_{22}^*\right)^{-1}\mathbf{R}_{22}^{-1}\mathbf{R}_{12}^T & -\mathbf{R}_{11}^* + \mathbf{R}_{12}^*\left(\mathbf{R}_{22}^{-1} - \mathbf{R}_{22}^*\right)^{-1}\mathbf{R}_{12}^\dagger \end{pmatrix}.$$

One can verify that the $\mathrm{tr}\rho = \frac{\sqrt{\det[\mathbf{I}+\mathbf{R}_{22}^{\dagger}\mathbf{R}_{22}]}}{\sqrt{\det[\mathbf{I}+\mathbf{R}^{\dagger}\mathbf{R}]}}\sqrt{\det[\boldsymbol{\Omega}]} = 1$, where we have put $\mathrm{Pf}[\boldsymbol{\mathcal{A}}] = \sqrt{\det[\boldsymbol{\mathcal{A}}]}$. Be noted that $\mathrm{Pf}[\cdots] = \pm\sqrt{\det[\cdots]}$ and if we write the coefficients in terms of Pfaffian then there is minus sign in case the system size is even and subsystem is odd.

In a general case where $\mathbf{R}$ is a complex matrix we have

$$\langle\boldsymbol{\xi}|\,\rho\,|\boldsymbol{\xi}'\rangle = |\mathcal{C}|^2\, e^{\sum_{i,j}\frac{1}{2}\mathcal{X}_{ij}\bar{\xi}_i\bar{\xi}_j} e^{\sum_{i,j}\mathcal{Y}_{ij}\bar{\xi}_i\xi'_j} e^{\sum_{i,j}-\frac{1}{2}\mathcal{X}^*_{ij}\xi'_i\xi'_j}; \tag{4.12}$$

with

$$\boldsymbol{\mathcal{X}} = \mathbf{R}_{11} - \mathbf{R}_{12}\boldsymbol{\mathcal{Q}}\mathbf{R}^*_{22}\mathbf{R}^T_{12} \qquad \text{and} \qquad 2\boldsymbol{\mathcal{Y}} = \mathbf{R}_{12}\boldsymbol{\mathcal{Q}}\mathbf{R}^{\dagger}_{12} + \mathbf{R}^*_{12}\boldsymbol{\mathcal{Q}}^*\mathbf{R}^T_{12}, \tag{4.13}$$

where $\boldsymbol{\mathcal{Q}} = \left(\mathbf{I} + {\mathbf{R}_{22}}^{\dagger}\mathbf{R}_{22}\right)^{-1}$ and $|\mathcal{C}|^2 = \frac{\sqrt{\det[\mathbf{I}+\mathbf{R}_{22}^{\dagger}\mathbf{R}_{22}]}^2}{\sqrt{\det[\mathbf{I}+\mathbf{R}^{\dagger}\mathbf{R}]}}$. If we assume that $\mathbf{R}$ is real ($\mathbf{R}^* = \mathbf{R}$), we could get a more compact form for equation (4.10).

$$\rho_{\mathbb{1}}(\boldsymbol{\xi},\boldsymbol{\xi}') = |\mathcal{C}|^2\, e^{\sum_{i,j}\frac{1}{2}\mathcal{X}_{ij}\bar{\xi}_i\bar{\xi}_j} e^{\sum_{i,j}\mathcal{Y}_{ij}\bar{\xi}_i\xi'_j} e^{\sum_{i,j}-\frac{1}{2}\mathcal{X}_{ij}\xi'_i\xi'_j}; \qquad i,j \le k \tag{4.14}$$

with

$$\boldsymbol{\mathcal{X}} = \mathbf{R}_{11} - \boldsymbol{\mathcal{Q}}\mathbf{R}_{22}\boldsymbol{\mathcal{Q}}^T \qquad \text{and} \qquad \boldsymbol{\mathcal{Y}} = \boldsymbol{\mathcal{Q}}\boldsymbol{\mathcal{Q}}^T, \tag{4.15}$$

where $\boldsymbol{\mathcal{Q}} = \mathbf{R}_{12}(\mathbf{I} - \mathbf{R}_{22})^{-1}$, and $|\mathcal{C}|^2 = \frac{\sqrt{\det[\mathbf{I}+\mathbf{R}_{22}^T\mathbf{R}_{22}]}}{\sqrt{\det[\mathbf{I}+\mathbf{R}^T\mathbf{R}]}}$.

The form above is really useful, one can reconstruct the operator form of the reduced density matrix. To derive the operator form for $\rho_{\mathbb{1}}$ from equation (4.14), using the relations $c_ic_j\,|\boldsymbol{\xi}\rangle = \xi_i\xi_j\,|\boldsymbol{\xi}\rangle$ and $\langle\boldsymbol{\xi}|\,c_i^{\dagger}c_j^{\dagger} = \langle\boldsymbol{\xi}|\,\bar{\xi}_i\bar{\xi}_j$, one can replace $\bar{\xi}_i\bar{\xi}_j$ with $c_i^{\dagger}c_j^{\dagger}$ and $\xi_{i\prime}\xi'_j$ with c_ic_j in the left and right exponentials equation (4.14). For the cross terms, one first diagonalizes the matrix $\mathbf{Y}$ then $\bar{\xi}_i\xi'_j$ can be rewritten with the relation

$$\mathcal{Y}_{ij}\bar{\xi}_i\xi'_j \;\rightarrow\; \ln(\boldsymbol{\mathcal{Y}})_{ij}c_i^{\dagger}c_j.$$

Therefore we have the operator form of RDM as

$$\rho_{\mathbb{1}} = |\mathcal{C}|^2\, e^{\sum_{i,j}\frac{1}{2}\mathcal{X}_{ij}c_i^{\dagger}c_j^{\dagger}} e^{\sum_{i,j}\ln(\boldsymbol{\mathcal{Y}})_{ij}c_i^{\dagger}c_j} e^{\sum_{i,j}-\frac{1}{2}\mathcal{X}^*_{ij}c_ic_j}. \tag{4.16}$$

Next, we can write the (4.16) as:

$$\rho_{\mathbb{1}} = |\mathcal{C}|^2\, e^{\frac{1}{2}\begin{pmatrix}\mathbf{c}^{\dagger} & \mathbf{c}\end{pmatrix}\boldsymbol{\mathcal{M}_1}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^{\dagger}\end{pmatrix}}\, e^{\frac{1}{2}\begin{pmatrix}\mathbf{c}^{\dagger} & \mathbf{c}\end{pmatrix}\boldsymbol{\mathcal{M}_2}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^{\dagger}\end{pmatrix}}\, e^{\frac{1}{2}\begin{pmatrix}\mathbf{c}^{\dagger} & \mathbf{c}\end{pmatrix}\boldsymbol{\mathcal{M}_3}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^{\dagger}\end{pmatrix}}\, e^{\frac{1}{2}\mathrm{tr}\ln(\boldsymbol{\mathcal{Y}})}, \tag{4.17}$$

where $\boldsymbol{\mathcal{M}_1}$, $\boldsymbol{\mathcal{M}_2}$ and $\boldsymbol{\mathcal{M}_3}$ are given by

$$\boldsymbol{\mathcal{M}_1} = \begin{pmatrix}\mathbf{0} & \boldsymbol{\mathcal{X}}\\ \mathbf{0} & \mathbf{0}\end{pmatrix}, \quad \boldsymbol{\mathcal{M}_2} = \begin{pmatrix}\ln(\boldsymbol{\mathcal{Y}}) & \mathbf{0}\\ \mathbf{0} & -\ln(\boldsymbol{\mathcal{Y}})\end{pmatrix}, \quad \boldsymbol{\mathcal{M}_3} = \begin{pmatrix}\mathbf{0} & \mathbf{0}\\ -\boldsymbol{\mathcal{X}}^* & \mathbf{0}\end{pmatrix}. \tag{4.18}$$

[2] we have used the expansion $(\mathbf{A}+\mathbf{B})^{-1} = \mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{B}\mathbf{A}^{-1} + \mathbf{A}^{-1}\mathbf{B}\mathbf{A}^{-1}\mathbf{B}\mathbf{A}^{-1} + \cdots$

These three matrices can be infused together into one matrix $\mathcal{M}$.

Therefore, it was possible to have a compact operator form for reduced density matrix as:

$$\rho_{\mathbb{1}} = |\mathcal{C}'|^2 \, e^{\frac{1}{2}\begin{pmatrix}\mathbf{c}^\dagger & \mathbf{c}\end{pmatrix}\boldsymbol{\mathcal{M}}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^\dagger\end{pmatrix}}, \quad \text{where} \quad e^{\boldsymbol{\mathcal{M}}} = e^{\boldsymbol{\mathcal{M}_1}} \, e^{\boldsymbol{\mathcal{M}_2}} \, e^{\boldsymbol{\mathcal{M}_3}}. \tag{4.19}$$

Where $|\mathcal{C}'|^2 = |\mathcal{C}|^2 \, e^{\frac{1}{2}\operatorname{tr}\ln(\boldsymbol{\mathcal{Y}})}$. For the simple case where $\mathbf{R}$ matrix is real, we can write

$$e^{\boldsymbol{\mathcal{M}}} = \boldsymbol{\mathcal{T}}, \qquad \text{where} \qquad \boldsymbol{\mathcal{T}} = \begin{pmatrix} \boldsymbol{\mathcal{Y}} - \boldsymbol{\mathcal{X}}\boldsymbol{\mathcal{Y}}^{-T}\boldsymbol{\mathcal{X}}^* & \boldsymbol{\mathcal{X}}\boldsymbol{\mathcal{Y}}^{-T} \\ -\boldsymbol{\mathcal{Y}}^{-T}\boldsymbol{\mathcal{X}}^* & \boldsymbol{\mathcal{Y}}^{-T} \end{pmatrix}. \tag{4.20}$$

equivalently, one can write $\boldsymbol{\mathcal{M}} = \ln(\boldsymbol{\mathcal{T}})$. Finally, since the Fermionic operators appear quadratic in the exponents above, $\rho_{\mathbb{1}}$ can be diagonalized, using Bogoliubov transformations.

The fermionic coherent state and Berezin integration on Grassmann variables proven to be a effective method to calculate RDM and correlations. When it is possible to write the state of the system in the Gaussian form of (2.51), then calculations in fermion coherent state are very useful. Although complicated at the first sight, the are many more complicated calculations that we have been able to preform with this method, as an example see [17] (equivalently chapter 7) or appendix D.

4.1.2 Density matrix for excited eigenstates

A typical excited eigenstate created by action creation operators on vacuum of η as (7.27).

$$|\psi\rangle = |k_1, k_2, \cdots, k_N\rangle = \prod_{k_j \in \mathbb{E}} \eta^\dagger_{k_j} \, |0\rangle \, . \tag{4.21}$$

Using equation (2.60) and the definition of the fermionic coherent state, we can write the density matrix for the excited eigenstate $|\psi\rangle$ as

$$\rho^\psi = |C^\psi|^2 e^{\frac{1}{2}\sum_{i,j} R^\psi_{ij} c^\dagger_i c^\dagger_j} \, |0\rangle_{c\,c}\langle 0| \, e^{-\frac{1}{2}\sum_{i,j} R^{\psi\,*}_{ij} c_i c_j}, \tag{4.22}$$

and C^ψ is given as (2.60). Similar to the density matrix for vacuum state we write the matrix form of density operator in terms of Grassmann variables using (A.16).

$$\rho^\psi(\boldsymbol{\xi}, \boldsymbol{\xi}') = \langle \boldsymbol{\xi}| \, \rho^\psi \, |\boldsymbol{\xi}'\rangle = |C^\psi|^2 \, e^{\frac{1}{2} R^\psi_{ij} \bar{\xi}_i \bar{\xi}_j} \, e^{-\frac{1}{2} R^{\psi\,*}_{ij} \xi'_i \xi'_j}. \tag{4.23}$$

The rest of the calculations in this part and the next are analogous to the subsection 4.1.1. For the next step, we divide the system into two subsystems $\mathbb{1}$ and $\mathbb{2}$ and trace out fermions in part $\mathbb{2}$.

$$\rho^\psi_{\mathbb{1}}(\boldsymbol{\xi}, \boldsymbol{\xi}') = |C^\psi|^2 e^{\frac{1}{2}(\mathbf{R}^\psi_{11})_{ij}\bar{\xi}_i\bar{\xi}_j - \frac{1}{2}(\mathbf{R}^{\psi\,*}_{11})_{ji}\xi'_j\xi'_i} \int \prod_{l\in\mathbb{2}} \mathrm{d}\bar{\xi}_l \mathrm{d}\xi_l \; e^{\frac{1}{2}\begin{pmatrix}\bar{\xi} & \xi\end{pmatrix}\boldsymbol{\mathcal{A}}^\psi\begin{pmatrix}\bar{\xi}\\ \xi\end{pmatrix} + \boldsymbol{\zeta}^\psi\boldsymbol{\xi} + \boldsymbol{\kappa}^\psi\bar{\boldsymbol{\xi}}} \tag{4.24}$$

where we have divided the $\mathbf{R}^{\psi}$ into four submatrices $\mathbf{R}^{\psi}_{\mathbf{11}}$, $\mathbf{R}^{\psi}_{\mathbf{12}}$, $\mathbf{R}^{\psi}_{\mathbf{21}}$ and $\mathbf{R}^{\psi}_{\mathbf{22}}$, according to the parts we are tracing out or not. The matrix $\boldsymbol{\mathcal{A}}^{\psi}$ can be thought of as a block matrix

$$\boldsymbol{\mathcal{A}}^{\psi} = \begin{pmatrix} \mathbf{R}^{\psi}_{22} & -\mathbf{I} \\ \mathbf{I} & -\mathbf{R}^{\psi\,*}_{22} \end{pmatrix}$$

In addition $\boldsymbol{\zeta}^{\psi} = -\boldsymbol{\xi}'\mathbf{R}^{\psi\,*}_{12}$ and $\boldsymbol{\kappa}^{\psi} = -\bar{\boldsymbol{\xi}}\mathbf{R}^{\psi}_{12}$. Now to calculate the partial trace we define new Grassmann variables $\boldsymbol{\eta}^T = \begin{pmatrix} \bar{\boldsymbol{\xi}} & \boldsymbol{\xi} \end{pmatrix}$ and

$$\boldsymbol{\lambda}^T = \begin{pmatrix} \boldsymbol{\kappa} & \boldsymbol{\zeta} \end{pmatrix} = \begin{pmatrix} \bar{\boldsymbol{\xi}} & \boldsymbol{\xi}' \end{pmatrix} \begin{pmatrix} -\mathbf{R}^{\psi}_{12} & \mathbf{0} \\ \mathbf{0} & -\mathbf{R}^{\psi\,*}_{12} \end{pmatrix}. \tag{4.25}$$

We denote those parts that are at the back of integral by $\mathcal{F}^{\psi}(\{\xi'_i\}, \{\bar{\xi}_j\})$. Now, for the reduced density matrix we have:

$$\rho^{\psi}_{\mathbb{1}}(\boldsymbol{\xi}, \boldsymbol{\xi}') = \mathcal{F}^{\psi}(\{\xi'_i\}, \{\bar{\xi}_j\}) \int \mathbf{D}\boldsymbol{\eta}\; e^{\frac{1}{2}\boldsymbol{\eta}^T \boldsymbol{\mathcal{A}}^{\boldsymbol{\psi}} \boldsymbol{\eta} + \boldsymbol{\lambda}^T \boldsymbol{\eta}} = \mathcal{F}^{\psi}(\{\xi'_i\}, \{\bar{\xi}_j\})\, \mathrm{Pf}[\boldsymbol{\mathcal{A}}^{\psi}] e^{\frac{1}{2}\boldsymbol{\lambda}^T \boldsymbol{\mathcal{A}}^{\boldsymbol{\psi}\,-1} \boldsymbol{\lambda}}. \tag{4.26}$$

We used the equation (A.7) to solve the integral. Putting it all together, we get for the reduced density matrix

$$\rho^{\psi}_{\mathbb{1}}(\boldsymbol{\xi}, \boldsymbol{\xi}') = \frac{\sqrt{\det\left[\mathbf{I} + \mathbf{R}^{\boldsymbol{\psi}\,\dagger}_{22} \mathbf{R}^{\boldsymbol{\psi}}_{22}\right]}}{\sqrt{\det\left[\mathbf{I} + \mathbf{R}^{\psi\dagger} \mathbf{R}^{\psi}\right]}} e^{\frac{1}{2}\begin{pmatrix} \bar{\xi} & \xi' \end{pmatrix} \boldsymbol{\Omega}^{\psi} \begin{pmatrix} \bar{\xi} \\ \xi' \end{pmatrix}} \tag{4.27}$$

where $\boldsymbol{\Omega}^{\psi}$ matrix is given by

$$\boldsymbol{\Omega}^{\psi} = \begin{pmatrix} \mathbf{R}^{\psi}_{11} & 0 \\ 0 & -\mathbf{R}^{\psi\,*}_{11} \end{pmatrix} + \begin{pmatrix} \mathbf{R}^{\psi}_{12} & 0 \\ 0 & \mathbf{R}^{\psi\,*}_{12} \end{pmatrix} \left(\boldsymbol{\mathcal{A}}^{\boldsymbol{\psi}}\right)^{-1} \begin{pmatrix} \mathbf{R}^{\psi\,T}_{12} & 0 \\ 0 & \mathbf{R}^{\psi\,\dagger}_{12} \end{pmatrix} \tag{4.28}$$

One can verify that the $\mathrm{tr}\rho^{\psi} = \frac{\sqrt{\det[\mathbf{I}+\mathbf{R}^{\boldsymbol{\psi}\,\dagger}_{22}\mathbf{R}^{\boldsymbol{\psi}}_{22}]}}{\sqrt{\det[\mathbf{I}+\mathbf{R}^{\psi\,\dagger}\mathbf{R}^{\psi}]}} \sqrt{\det[\boldsymbol{\Omega}^{\psi}]} = 1$. One can reconstruct the operator form of the reduced density matrix for an excited state by going through the same process as previous subsection. Therefore, we get

$$\rho^{\psi}_{\mathbb{1}} = \mathcal{C}^{\psi}\, e^{\sum_{i,j} \frac{1}{2}\mathcal{X}^{\psi}_{ij} c^{\dagger}_i c^{\dagger}_j} e^{\sum_{i,j} \ln(\boldsymbol{\mathcal{Y}}^{\boldsymbol{\psi}})_{ij} c^{\dagger}_i c_j} e^{\sum_{i,j} -\frac{1}{2}\mathcal{X}^{\boldsymbol{\psi}\,*}_{ij} c_i c_j}. \tag{4.29}$$

with

$$\boldsymbol{\mathcal{X}}^{\boldsymbol{\psi}} = \mathbf{R}^{\boldsymbol{\psi}}_{11} - \mathbf{R}^{\boldsymbol{\psi}}_{12} \boldsymbol{\mathcal{Q}}^{\boldsymbol{\psi}} \mathbf{R}^{\boldsymbol{\psi}\,*}_{22} \mathbf{R}^{\boldsymbol{\psi}\,T}_{12} \tag{4.30a}$$

$$2\boldsymbol{\mathcal{Y}}^{\boldsymbol{\psi}} = \mathbf{R}^{\boldsymbol{\psi}}_{12} \boldsymbol{\mathcal{Q}}^{\boldsymbol{\psi}} \mathbf{R}^{\boldsymbol{\psi}\,\dagger}_{12} + \mathbf{R}^{\boldsymbol{\psi}\,*}_{12} \boldsymbol{\mathcal{Q}}^{\boldsymbol{\psi}*} \mathbf{R}^{\boldsymbol{\psi}\,T}_{12}, \tag{4.30b}$$

$$\boldsymbol{\mathcal{Q}}^{\boldsymbol{\psi}} = \left(\mathbf{I} + \mathbf{R}^{\boldsymbol{\psi}\,\dagger}_{22} \mathbf{R}^{\boldsymbol{\psi}}_{22}\right)^{-1} \qquad \text{and} \quad \mathcal{C}^{\psi} = \frac{\sqrt{\det\left[\mathbf{I} + \mathbf{R}^{\boldsymbol{\psi}\,\dagger}_{22} \mathbf{R}^{\boldsymbol{\psi}}_{22}\right]}}{\sqrt{\det\left[\mathbf{I} + \mathbf{R}^{\psi\dagger} \mathbf{R}^{\psi}\right]}} \tag{4.30c}$$

4.2 Majorana representation of reduced density matrix

In this section, we write the reduced density matrix of a state which follows Wick's theorem. Then because of Gaudin's theorem, most of the states can be written in a Gaussian form so one can make the following ansatz for the reduced density matrix of the domain D:

$$\rho_D = \frac{1}{Z_D} e^{\mathcal{O}}, \tag{4.31}$$

where we assumed $\mathcal{O}$ is in the quadratic Majorana operator form and $Z_D = \prod_k 2\cosh\frac{d_k}{2}$ is the normalization constant. By definition, if ρ_D is the reduced density matrix the correlation functions inside the domain should match those that one calculates using the state of the full system. First, we write the reduced density matrix as follows:

$$\rho_D = \prod_k \frac{e^{-\frac{d_k}{2}} + 2\sinh\frac{d_k}{2}\delta_k^\dagger\delta_k}{2\cosh\frac{d_k}{2}}. \tag{4.32}$$

Then it is easy to show that

$$\langle\delta_k^\dagger\delta_{k'}\rangle = \frac{\delta_{kk'}}{1+e^{-\frac{d_k}{2}}}, \qquad \langle\delta_k\delta_{k'}\rangle = 0. \tag{4.33}$$

Using the above we can calculate the $\mathbf{\Gamma}$ correlation function which has the following form:

$$\mathbf{\Gamma} = \tanh\frac{\mathbf{W}}{2}. \tag{4.34}$$

At this stage we can also write the equation (4.32) for the eigenvalues of the $\mathbf{\Gamma}$ matrix, i.e. ν's as follows:

$$\rho_D = \prod_k \left(\frac{1-\nu_k}{2} + \nu_k\delta_k^\dagger\delta_k\right) = \prod_k \left(\frac{1+\nu_k}{2}\delta_k^\dagger\delta_k + \frac{1-\nu_k}{2}\delta_k\delta_k^\dagger\right) \tag{4.35}$$

Finally the reduced density matrix can be also written as:

$$\rho_D = [\det\frac{I-\mathbf{\Gamma}}{2}]^{\frac{1}{2}} e^{\frac{1}{2}(\gamma\ \ \bar{\gamma}).\ln\frac{I+\mathbf{\Gamma}}{I-\mathbf{\Gamma}}.\begin{pmatrix}\gamma\\ \bar{\gamma}\end{pmatrix}}, \tag{4.36}$$

where we have

$$\det[\frac{I-\mathbf{\Gamma}}{2}] = \det\mathbf{K}.\det[\frac{\bar{\mathbf{K}} - \mathbf{G}.\mathbf{K}^{-1}.\mathbf{G}^T}{2}], \tag{4.37}$$

One can also come back and write the argument of the exponential in the original fermion representation as follows:

$$\rho_D = [\det\frac{I-\mathbf{\Gamma}}{2}]^{\frac{1}{2}} e^{\frac{1}{2}(\mathbf{c}^\dagger\ \ \mathbf{c})\mathbf{M}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^\dagger\end{pmatrix}}, \tag{4.38}$$

where

$$\mathbf{M} = \begin{pmatrix} \mathbf{P} & \mathbf{Q} \\ -\mathbf{Q}^* & -\mathbf{P}^* \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} I & iI \\ I & -iI \end{pmatrix} . \mathbf{W} . \frac{1}{\sqrt{2}} \begin{pmatrix} I & I \\ -iI & iI \end{pmatrix}, \tag{4.39}$$

and I have renamed the following

$$\mathbf{W} = \begin{pmatrix} \mathbf{W}_{11} & \mathbf{W}_{12} \\ \mathbf{W}_{21} & \mathbf{W}_{22} \end{pmatrix} = \ln \frac{I + \mathbf{\Gamma}}{I - \mathbf{\Gamma}}. \tag{4.40}$$

Since we have:

$$\frac{1}{\sqrt{2}} \begin{pmatrix} I & iI \\ I & -iI \end{pmatrix} . \frac{1}{\sqrt{2}} \begin{pmatrix} I & I \\ -iI & iI \end{pmatrix} = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}. \tag{4.41}$$

We can take these matrices inside the ln and then define

$$\tilde{\mathbf{\Gamma}} = \frac{1}{\sqrt{2}} \begin{pmatrix} I & iI \\ I & -iI \end{pmatrix} . \mathbf{\Gamma} . \frac{1}{\sqrt{2}} \begin{pmatrix} I & I \\ -iI & iI \end{pmatrix}. \tag{4.42}$$

Then finally we will have:

$$\rho_D = [\det \frac{\mathbf{I} - \mathbf{\Gamma}}{2}]^{\frac{1}{2}} e^{\frac{1}{2}(\mathbf{c}^\dagger \ \mathbf{c}) \ln \frac{\mathbf{I}+\mathbf{\Gamma}}{\mathbf{I}-\mathbf{\Gamma}} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix}}, \tag{4.43}$$

When all the couplings are real like when we are dealing with the eigenstate of a Hamiltonian with real couplings the reduced density matrix can be written as:

$$\rho_D = \det[\frac{1}{2}(\mathbf{I} - \mathbf{G})] e^{\mathcal{H}}, \tag{4.44}$$

$$\mathcal{H} = \frac{1}{2}(\mathbf{c}^\dagger \ \mathbf{c}) \begin{pmatrix} \mathbf{M} & \mathbf{N} \\ -\mathbf{N} & -\mathbf{M} \end{pmatrix} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix} + \frac{1}{2} \mathrm{Tr} \ln (\mathbf{F}_s), \tag{4.45}$$

where $\mathcal{H}$ is the entanglement Hamiltonian and

$$\begin{pmatrix} \mathbf{M} & \mathbf{N} \\ \mathbf{-N} & \mathbf{-M} \end{pmatrix} = \ln \begin{pmatrix} \mathbf{F}_s - \mathbf{F}_a \mathbf{F}_s^{-1} \mathbf{F}_a & \mathbf{F}_a \mathbf{F}_s^{-1} \\ -\mathbf{F}_s^{-1} \mathbf{F}_a & \mathbf{F}_s^{-1} \end{pmatrix}, \tag{4.46}$$

where $\mathbf{F}_a = \frac{\mathbf{F}-\mathbf{F}^T}{2}$ and $\mathbf{F}_s = \frac{\mathbf{F}+\mathbf{F}^T}{2}$ and as before $\mathbf{F} = \frac{\mathbf{I}+\mathbf{G}}{\mathbf{I}-\mathbf{G}}$. When the $\mathbf{G}$ matrix is real and symmetric one can write everything with respect to the $\mathbf{C}$ matrix as follows:

$$\rho_D = \det[\mathbf{I} - \mathbf{C}] e^{c_i^\dagger (\ln \mathbf{F})_{ij} c_j}, \tag{4.47}$$

where $\mathbf{F} = \frac{\mathbf{C}}{\mathbf{I}-\mathbf{C}}$.

4.3 Density matrix for a general state

To study the entanglement content of a general defined in subsection 2.3.5, first one should create the density matrix for such a state. The density matrix of state $|\varphi\rangle$ (2.71) has the form

$$\begin{aligned}\rho^{\varphi} =& \sum_{r,s} a_r a_s^* \left|E_r\right\rangle \left\langle E_s\right| = \sum_{r} \left|a_r\right|^2 \left|E_r\right\rangle \left\langle E_r\right| + \sum_{r\neq s} a_r a_s^* \left|E_r\right\rangle \left\langle E_s\right| \\ =& \sum_{r} \left|a_r\right|^2 \rho^r + \sum_{r\neq s} a_r a_s^* \varrho^{rs}\end{aligned} \tag{4.48}$$

The first term is the sum of the density matrix of excited eigenstates and the second term is the sum of *cross density* terms ϱ^{rs}. We already studied the excited density matrices in subsection 4.1.2, in this part we want to focus on the cross terms ϱ^{rs}. We can use the same method Introduced in subsections 4.1.2 and 4.1.1 to write the (reduced) cross density matrix for a general state.

$$\varrho^{rs} = C^{rs} e^{\frac{1}{2} R^r_{ij} c_i^\dagger c_j^\dagger} \left|0\right\rangle_{c\,c}\!\left\langle 0\right| e^{-\frac{1}{2} R^{s\,*}_{ij} c_i c_j} \tag{4.49}$$

where $\mathbb{E}_r$ and $\mathbb{E}_s$ are two unequal sets of excited modes. Essentially, these two sets do not have the same length. However, we have assumed that the state $|\varphi\rangle$ is an eigenstate of parity operator. Also

$$C^{rs} = \frac{1}{(\det[\mathbf{I} + \mathbf{R^{r\dagger}R^r}])^{\frac{1}{4}} (\det[\mathbf{I} + \mathbf{R^{s\dagger}R^s}])^{\frac{1}{4}}}. \tag{4.50}$$

Now we write the matrix form of this cross density operator in terms of Grassmann variables using (A.16).

$$\varrho^{rs}(\boldsymbol{\xi}, \boldsymbol{\xi'}) = \left\langle \boldsymbol{\xi}\right| \varrho^{rs} \left|\boldsymbol{\xi'}\right\rangle = \left|C^{rs}\right|^2 e^{\frac{1}{2} R^r_{ij} \bar{\xi}_i \bar{\xi}_j} \; e^{-\frac{1}{2} R^{s\,*}_{ij} \xi'_i \xi'_j}. \tag{4.51}$$

Similar to the calculations of subsections 4.1.1 and 4.1.2. For the next step, we divide the system into two subsystems $\mathbb{1}$ and $\mathbb{2}$ and trace out fermions in part $\mathbb{2}$.

$$\varrho^{rs}_{\mathbb{1}}(\boldsymbol{\xi}, \boldsymbol{\xi'}) = C^{rs} e^{\frac{1}{2} (\mathbf{R}^r_{11})_{ij} \bar{\xi}_i \bar{\xi}_j - \frac{1}{2} (\mathbf{R}^{s\,*}_{11})_{ji} \xi'_j \xi'_i} \int \prod_{l\in\mathbb{2}} \mathrm{d}\bar{\xi}_l \mathrm{d}\xi_l \; e^{\frac{1}{2} \begin{pmatrix} \bar{\xi} & \xi \end{pmatrix} \boldsymbol{\mathcal{A}^{rs}} \begin{pmatrix} \bar{\xi} \\ \xi \end{pmatrix} + \boldsymbol{\zeta}^s \boldsymbol{\xi} + \boldsymbol{\kappa}^r \bar{\boldsymbol{\xi}}}. \tag{4.52}$$

where matrix $\boldsymbol{\mathcal{A}^{rs}}$ is a block matrix made from submatrices of $\mathbf{R}^r$ and $\mathbf{R}^s$.

$$\boldsymbol{\mathcal{A}^{rs}} = \begin{pmatrix} \mathbf{R^r_{22}} & -\mathbf{I} \\ \mathbf{I} & -\mathbf{R^{s\,*}_{22}} \end{pmatrix}$$

In addition $\boldsymbol{\zeta}^s = -\boldsymbol{\xi'} \mathbf{R^{s\,*}_{12}}$ and $\boldsymbol{\kappa^r} = -\bar{\boldsymbol{\xi}} \mathbf{R^r_{12}}$. We have divided our $\mathbf{R}^r$ and $\mathbf{R}^s$ matrices into four submatrices according to the parts we are tracing out or not. If we denote those parts that are at the back of integral by $\mathcal{F}^{rs}(\{\xi'_i\}, \{\bar{\xi}_j\})$. Now, to calculate the partial trace we

define new Grassmann variables $\boldsymbol{\eta}^T = \begin{pmatrix}\bar{\boldsymbol{\xi}} & \boldsymbol{\xi}\end{pmatrix}$ and $\boldsymbol{\lambda}^T = \begin{pmatrix}\boldsymbol{\kappa} & \boldsymbol{\zeta}\end{pmatrix}$. Using equation (A.7), for reduced density matrix we have:

$$\varrho_{\mathbb{1}}^{rs}(\boldsymbol{\xi},\boldsymbol{\xi}') = \mathcal{F}^{rs}(\{\xi_i'\},\{\bar{\xi}_j\}) \int \mathbf{D}\boldsymbol{\eta}\; e^{\frac{1}{2}\boldsymbol{\eta}^T\boldsymbol{\mathcal{A}}^{\boldsymbol{rs}}\boldsymbol{\eta}+\boldsymbol{\lambda}^T\boldsymbol{\eta}} = \mathcal{F}^{rs}(\{\xi_i'\},\{\bar{\xi}_j\})\,\mathrm{Pf}[\boldsymbol{\mathcal{A}}^{\boldsymbol{rs}}] e^{\frac{1}{2}\boldsymbol{\lambda}^T(\boldsymbol{\mathcal{A}}^{\boldsymbol{rs}})^{-1}\boldsymbol{\lambda}}. \tag{4.53}$$

Putting it all together, we get for the reduced cross density matrix

$$\varrho_1^{rs}(\boldsymbol{\xi},\boldsymbol{\xi}') = \frac{\sqrt{\det\left[\mathbf{I}+\mathbf{R}_{22}^{\mathbf{s}\,\dagger}\mathbf{R}_{22}^{\mathbf{r}}\right]}}{\sqrt[4]{\det\left[\mathbf{I}+\mathbf{R}^{\mathbf{r}\dagger}\mathbf{R}^{\mathbf{r}}\right]}\sqrt[4]{\det\left[\mathbf{I}+\mathbf{R}^{\mathbf{s}\dagger}\mathbf{R}^{\mathbf{s}}\right]}} e^{\frac{1}{2}\begin{pmatrix}\bar{\xi} & \xi'\end{pmatrix}\boldsymbol{\Omega}^{\mathbf{rs}}\begin{pmatrix}\bar{\xi}\\ \xi'\end{pmatrix}} \tag{4.54}$$

where $\boldsymbol{\Omega}^{\boldsymbol{rs}}$ matrix is given by

$$\boldsymbol{\Omega}^{\boldsymbol{rs}} = \begin{pmatrix}\mathbf{R}_{11}^{\mathbf{r}} & 0\\ 0 & -\mathbf{R}_{11}^{\mathbf{s}\,*}\end{pmatrix} + \begin{pmatrix}\mathbf{R}_{12}^{\mathbf{r}} & 0\\ 0 & \mathbf{R}_{12}^{\mathbf{s}\,*}\end{pmatrix}\left(\boldsymbol{\mathcal{A}}^{\boldsymbol{rs}}\right)^{-1}\begin{pmatrix}\mathbf{R}_{12}^{\mathbf{r}\,T} & 0\\ 0 & \mathbf{R}_{12}^{\mathbf{s}\,\dagger}\end{pmatrix} \tag{4.55}$$

One can verify that the $\mathrm{tr}\varrho^{rs} = 0$. To reconstruct the operator form of the reduced cross density matrix for an excited state we go through the same process as in previous subsections. Therefore, we get

$$\varrho_{\mathbb{1}}^{rs} = \mathcal{C}^{rs}\, e^{\sum_{i,j}\frac{1}{2}\mathcal{X}_{ij}^{rs}c_i^\dagger c_j^\dagger} e^{\sum_{i,j}\ln(\boldsymbol{\mathcal{Y}}^{\boldsymbol{rs}})_{ij}c_i^\dagger c_j} e^{\sum_{i,j}\frac{1}{2}\mathcal{Z}_{ij}^{rs}c_i c_j}. \tag{4.56}$$

with

$$\boldsymbol{\mathcal{X}}^{\boldsymbol{rs}} = \boldsymbol{\Omega}_{11}^{\mathbf{rs}}, \qquad \boldsymbol{\mathcal{Z}}^{\boldsymbol{rs}} = \boldsymbol{\Omega}_{22}^{\mathbf{rs}} \qquad \text{and} \qquad 2\boldsymbol{\mathcal{Y}}^{\boldsymbol{rs}} = \boldsymbol{\Omega}_{12}^{\mathbf{rs}} - \boldsymbol{\Omega}_{21}^{\mathbf{rs}\,T} \tag{4.57a}$$

$$\mathcal{C}^{rs} = \frac{\sqrt{\det\left[\mathbf{I}+\mathbf{R}_{22}^{\mathbf{s}\,\dagger}\mathbf{R}_{22}^{\mathbf{r}}\right]}}{\sqrt[4]{\det\left[\mathbf{I}+\mathbf{R}^{\mathbf{r}\dagger}\mathbf{R}^{\mathbf{r}}\right]}\sqrt[4]{\det\left[\mathbf{I}+\mathbf{R}^{\mathbf{s}\dagger}\mathbf{R}^{\mathbf{s}}\right]}} \tag{4.57b}$$

— 5 —

Entanglement

Entanglement is a type of correlation between subsystems, which cannot be explained by classical physics. It is the central concept of quantum information theory and corresponds to the possibility of transmitting quantum information, that cannot be simulated by classical channels. For instance quantum teleportation [59] or quantum cryptography [60]. The problem of measuring and quantifying quantum correlations, or entanglement, in manybody quantum systems is a field of research on its own, that benefits both from condensed matter and quantum information developments. Here, I only discuss the von Neumann entropy and Rényi entanglement entropy as a measure for entanglement. Nevertheless, there are many other measures and a detailed review of them can be found in references [12, 61, 62, 63, 64]. In quantum many-body physics, entanglement entropy can be used to describe the properties (such as universality class or central charge) of the quantum phase transition in the model [65, 66].

First to answer the question “Is a state entangled or not?", we need a mathematical definition for entanglement versus separability. This is very simple for pure states: a pure state $|\psi\rangle$ is called *separable* if and only if it can be written as $|\psi\rangle = |\varphi_1\rangle \otimes |\varphi_2\rangle\ |\rangle \otimes \cdots \otimes |\varphi_N\rangle$, otherwise it is *entangled*. In other words, an **entangled** state is defined to be one whose quantum state cannot be factored as a product of states of its particles; Entanglement can happen when we have two or more particles, for example for a quantum system with two spins we can have:

$$\textbf{Not Entangled:} \begin{cases} |\psi_1\rangle = |\uparrow\rangle \otimes |\uparrow\rangle \\ \\ |\psi_2\rangle = \frac{|\downarrow\rangle \otimes (|\uparrow\rangle \pm |\downarrow\rangle)}{\sqrt{2}} \end{cases} \qquad \textbf{Entangled:} \begin{cases} |\psi_3\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle \pm |\downarrow\downarrow\rangle) \\ \\ |\psi_4\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle) \end{cases} \tag{5.1}$$

Note that throughout most of this thesis, we talk about the bipartite entanglement of a pure state.

I only consider the bipartition entanglement in manybody system or equivalently, dividing the system into two distinct regions A and B. If the total system is in a pure state then a measure of the entanglement between A and B is associated with the reduced density matrix of one of the two blocks, $S(A \text{ or } B)$. In studying the properties of entanglement entropy it is worth mentioning its dependence on the properties of the subsystems A and/or B. In a 1-dimensional system, the entanglement entropy of an eigenstate of the system (ground state or excited state) behaves as:

- Logarithmic law, which the entanglement grows logarithmically with the size of subsystem, $S(l) \approx \log(l)$.
- Area law, which the value of entanglement grows with the boundary points of the subsystem, $S(l) \approx$ #boundary points

- Volume law, which the entanglement grows linearly with the size of subsystem, $S(l) \approx \alpha l$

In the rest, I explain better the formulation of measures of the entanglement which has been used here. Also, we present formulas that one can calculate the entanglement entropy for the eigenstates of free fermions in terms of correlation matrices of the state. These methods are efficient and computationally easy, which is why they are vastly used. Some simple cases have been used as examples for better understanding of concepts.

5.1 Rényi Entanglement Entropy

The Rényi entanglement entropy is defined as follows:

$$S_\alpha = \frac{1}{1-\alpha} \ln \mathrm{tr}\rho^\alpha. \tag{5.2}$$

where ρ stands for the reduced density matrix of the subsystem. For a general quantum manybody state, the difficulty of calculation of the entanglement grows exponentially with the size of the subsystem. One can find a basis in which RDM is diagonal, however, it would still be computationally disadvantageous. However, it is possible to have a special structure for the RDM to simplify the entanglement calculation. For instance, having a Gaussian form for RDM simplifies the calculation, or being able to write the RDM in terms of correlation matrices [65, 67, 68, 69].

The first simplification can be the $\mathrm{tr}\rho^\alpha$ in(5.2) which can be calculated easily by using the trace formula

$$\mathrm{tr} e^{\frac{1}{2}\begin{pmatrix}\mathbf{c}^\dagger & \mathbf{c}^\dagger\end{pmatrix}\mathbf{M}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^\dagger\end{pmatrix}} = \det[\mathbf{I} + e^{\mathbf{M}}]^{\frac{1}{2}}. \tag{5.3}$$

Using the result of chapter 4 and writing the RDM in terms of correlation matrix $\mathbf{\Gamma}$, then we have:

$$\mathrm{tr}\rho^\alpha = \left(\det[\left(\frac{I-\mathbf{\Gamma}}{2}\right)^\alpha + \left(\frac{I+\mathbf{\Gamma}}{2}\right)^\alpha]\right)^{\frac{1}{2}} \tag{5.4}$$

Finally we have:

$$S_\alpha = \frac{1}{1-\alpha}\sum_\nu \ln[(\frac{1-\nu}{2})^\alpha + (\frac{1+\nu}{2})^\alpha], \tag{5.5}$$

where the sum is over all the positive eigenvalues of the purely imaginary skew-symmetric matrix $\mathbf{\Gamma}$.

The von Neumann entanglement entropy (S_{vN}), commonly called entanglement entropy, is given by the limit $\alpha \to 1^+$ of Rényi EE,

$$S_{vN}(A) = \lim_{\alpha\to 1^+} S_\alpha. \tag{5.6}$$

To find the expression for von Neumann entropy, we use the fact that S_α is differentiable in the region $\alpha > 1$, and hence the von Neumann entanglement entropy can be obtained as [39]:

$$S_{vN}(A) = \lim_{\alpha \to 1^+} \frac{\partial}{\partial \alpha} S_\alpha = -\mathrm{tr}_A[\rho_A \log \rho_A]. \tag{5.7}$$

There are many properties common to both Rényi entropy and the entanglement entropy, for more details see [70, 71]. The von Neumann entanglement entropy can also be computed with the following relation:

$$S_{vN} = -\sum_\nu (\frac{1-\nu}{2}) \ln[\frac{1-\nu}{2}] + (\frac{1+\nu}{2}) \ln[\frac{1+\nu}{2}]. \tag{5.8}$$

When all the couplings in the Hamiltonian are real, using (3.6) and (3.7), we can again write everything with respect to the matrix $\mathbf{G}$ as follows:

$$S_\alpha = \frac{1}{1-\alpha} \mathrm{tr} \ln \left(\frac{I - \sqrt{\mathbf{G}^T \mathbf{G}}}{2} \right)^\alpha + \left(\frac{I + \sqrt{\mathbf{G}^T \mathbf{G}}}{2} \right)^\alpha] \Big) \tag{5.9}$$

Finally, when the matrix $\mathbf{G}$ is symmetric we can write

$$S_\alpha = \frac{1}{1-\alpha} \mathrm{tr} \ln [\Big(I - \mathbf{C} \Big)^\alpha + \mathbf{C}^\alpha]. \tag{5.10}$$

The above formulas can be used to calculate bipartite entanglement entropy of the ground state or any excited eigenstates of the quadratic Hamiltonians.

Parte II

Publication

— 6 —

Bipartite entanglement entropy of the excited states of the free fermions

Bipartite entanglement entropy of quantum many-body systems exhibits a wide variety of interesting properties with a myriad of applications in high-energy and condensed matter physics. Some of the earliest studies were the calculation of the entanglement entropy of the ground state (GS) of the coupled harmonic oscillators and the establishment of the area-law in the same models in [72, 73, 74]. In Ref [75], the same quantity was calculated for the ground state of the conformal field theories (CFT) and the famous logarithmic-law with the central charge as the coefficient of the logarithm was derived. These studies were followed with many other interesting results which paved the way to better understanding of the bipartite entanglement entropy of the ground state of the free fermions [13, 14, 76], coupled harmonic oscillators [77, 78, 79], quantum spin chains [65, 67, 80], CFTs [81] and topological systems[82, 83]. To review various applications of the bipartite entanglement entropy of the ground state in many-body quantum systems and quantum field theories see [12, 84, 85, 69, 86, 87, 88, 89] and [8, 90, 91] respectively. Although the investigation of the bipartite entanglement entropy of the ground state of quantum systems has a long history the same is not true for the excited states. The bipartite entanglement entropy of the excited states in the quantum spin chains was first studied with exact methods in [92], see also [93]. Then the entanglement entropy of the low-lying excited states in CFTs was calculated in [94, 95]. For recent numerical calculations regarding the entanglement entropy of the excited states in the quantum spin chains and free fermions see [96, 97, 98, 99, 100, 101, 102, 47, 103, 104, 105, 106, 107, 108, 109, 110]. For further results on the entanglement entropy of the low-lying excited states in CFTs see [111, 112, 113, 114, 115, 116, 117]. Recently, there have also been analytical calculations regarding the quantum entanglement content of the quasi-particle excitations in massive field theories and integrable chains[118, 119].

It is widely believed that one expects universality and quantum field theory for the ground state (and low-lying excited states) of the quantum many-body systems at and around quantum phase transition point. This has been one of the reasons that most of the studies were focused on the bipartite entanglement entropy of the ground states. Nevertheless, some typical behaviors (volume-law) have been already observed for the excited states too, see Refs [97, 98, 99]. Some further analytical and numerical results were also obtained for the average of the entanglement entropy in [102, 106, 107] which support some sort of universality. In this chapter, we would like to study the entanglement content of the excited states of the generic translational invariant one dimensional free fermions. The quantity of interest is the von Neumann entropy which is defined for a system by partitioning it to A and $\bar{A}$, where A has l contiguous sites, and $\bar{A}$ has $L-l$ sites where we will occasionally send L to infinity. The von-Neumann entropy is

$$S_{vN} = -\mathrm{tr}\rho_l \ln \rho_l, \tag{6.1}$$

where ρ_l is the reduced density matrix of the part A. Although here the focus is on the von

Neumann entropy, one can almost trivially extend these results to Rényi entropies. For the ground state of the gapped systems S_{vN} saturates with the size of the subsystem[80], this is called an area-law. For the short-range critical one dimensional systems we have logarithmic-law [75, 81], i.e.

$$S_{vN} = \frac{c}{3} \ln \left[\frac{L}{\pi} \sin[\frac{\pi l}{L}] \right] + \text{const}, \tag{6.2}$$

where c is the central charge of the underlying CFT. When the S_{vN} changes linearly with l as happens typically for the excited states, we call it a volume-law. Most notably for one dimensional free fermions, we prove the followings: (1) All the Hamiltonians (independent of having a gap or not) have a lot of non-low lying excited states that can be described by CFT and have an arbitrary integer central charge. For free fermions sometimes we can also have excited states with half-integer central charges. (2) The degenerate excited states depending on the chosen subspace basis can follow volume-law, logarithmic-law and sometimes even an area-law. (3) For free fermions (and corresponding spin chains) there is a set of Hamiltonians that the ground state of every generic free fermion is one of the eigenstates of these Hamiltonians. In other words, one can find the ground state of a generic Hamiltonian as one of the eigenstates of these Hamiltonians. Excited states with integer central charges have been realized before in the context of the XX chain in [92], see also [93]. However, the results of this part can be extend to the generic translational invariant free fermions and coupled harmonic oscillators [16]. In addition, our simple method not only explains the existence of these kinds of excited states it also gives a natural way to make some statements regarding the average entanglement entropy studied in [102, 106, 107]. In particular, combining the result of [102] with a duality relation introduced in [120] we discover a method to calculate the average bipartite entanglement entropy over all the eigenstates of a generic free fermion Hamiltonian using a single eigenstate of the XX-chain with just a simple hopping coupling. Using this mapping instead of studying an exponential number of states one can just work with a *single* state which makes the previously considered unmeasurable quantity quite accessible for the experimental study.

This chapter is organized as follows: In section II, we first define the Hamiltonian of generic translational invariant free fermions. Then for later arguments, we present some integrals of motion of these Hamiltonians. To clarify the argument, we then consider the XX chain and prove some statements regarding the entanglement content of this model. After that, we extend our arguments to the general free fermions. Then we comment on the average entanglement over the excited states of free fermions, the role of the degeneracies, and how to measure specific averaging introduced in [102]. I encourage the interested reader to look at [16], where we have studied the bipartite entanglement entropy of the excited states for generic coupled harmonic oscillators as well.

6.1 Generic free fermions

In this section we discuss some generic properties of the entanglement entropy of the excited states of the one dimensional free fermions. The Hamiltonian of a translational invariant (periodic) free fermions with time-reversal symmetry can be written as

$$H = \sum_{r=-R}^{R} \sum_{j\in\Lambda} a_r c_j^\dagger c_{j+r} + \frac{b_r}{2}(c_j^\dagger c_{j+r}^\dagger - c_j c_{j+r}) + \text{const}, \tag{6.3}$$

with $\Lambda = \{1, 2, \cdots, L\}$. Using the Majorana operators $\gamma_j = c_j + c_j^\dagger$ and $\bar{\gamma}_j = i(c_j^\dagger - c_j)$ one can write $H = \frac{i}{2}\sum_{r=-R}^{R}\sum_{j\in\Lambda} t_r \bar{\gamma}_j \gamma_{j+r}$, where $t_r = -(a_r + b_r)$ and $t_{-r} = -(a_r - b_r)$. It is very useful to put the coupling constants as the coefficients of the following holomorphic function $f(z) = \sum_r t_r z^r$, see[121]: Then the Hamiltonian can be diagonalized by going to the Fourier space and then Bogoliubov transformation as follows:

$$H = \sum_k |f(k)| \eta_k^\dagger \eta_k + \text{const}, \tag{6.4}$$

where $\eta_k = \frac{1}{2}(1 + \frac{f(k)}{|f(k)|})c_k^\dagger + \frac{1}{2}(1 - \frac{f(k)}{|f(k)|})c_{-k}$ with $f(k) := f(e^{ik})$, where $k := \frac{2\pi}{L}j$ with $j = 1, 2, ..., L$. When the system is critical it is well-known that the number of zeros of the complex function $f(k)$ on the unit circle is twice the central charge of the underlying CFT. This will be our guiding principle in most of the upcoming discussions. The local mutually commuting integrals of motions can be written as follows:

$$I_n^+ = \sum_k \cos(nk)|f(k)|\eta_k^\dagger \eta_k, \qquad n = 0, 1, ..., \frac{L-1}{2}, \tag{6.5}$$

$$I_m^- = \sum_k \sin(mk)\eta_k^\dagger \eta_k, \qquad m = 1, ..., \frac{L-1}{2}. \tag{6.6}$$

The interesting and crucial fact is that the second set of integrals of motions in the real space can be written as

$$I_m^- = \frac{i}{2}\sum_{j\in\Lambda}(c_j^\dagger c_{j+m} - c_{j+m}^\dagger c_j), \tag{6.7}$$

which is independent of the parameters of the Hamiltonian. The above considerations are also correct if one uses Jordan-Wigner transformation and find the quantum spin chain equivalent of the above Hamiltonians and integrals of motion, see Appendix A. For example, all the periodic quantum spin chains that can be mapped to the free fermions commute with the following integrals of motion

$$I_m^-(XY) = \sum_{j\in\Lambda}\left[\sigma_j^x \sigma_{j+1}^z ... \sigma_{j+m-1}^z \sigma_{j+m}^y - \sigma_j^y \sigma_{j+1}^z ... \sigma_{j+m-1}^z \sigma_{j+m}^x\right], \tag{6.8}$$

which is independent of the parameters of the Hamiltonian.

To introduce the main idea we first start with the XX-chain with the following Hamiltonian

$$H_{XX} = -\sum_{j\in\Lambda}(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j). \tag{6.9}$$

We are interested in the structure of particular excited states in the spectrum of the above Hamiltonian. The local commuting integrals of motions after a bit of rearrangement are

$$I_n^+(XX) = -2\sum_k \cos(nk)\eta_k^\dagger\eta_k, \quad n = 0, 1, ..., \frac{L-1}{2}, \tag{6.10}$$

$$I_m^-(XX) = 2\sum_k \sin(mk)\eta_k^\dagger\eta_k, \quad m = 1, ..., \frac{L-1}{2}. \tag{6.11}$$

In the real space $I_n^-(XX)$ is (6.7) and $I_n^+(XX)$ has the following form:

$$I_n^+(XX) = -\sum_{j\in\Lambda}(c_j^\dagger c_{j+n} + c_{j+n}^\dagger c_j). \tag{6.12}$$

The Hamiltonian and the integrals of motion share a common eigenbasis. That means, for example, the ground state of $I_n^+(XX)$ appears as the excited state of H_{XX}. We use this basic fact to prove our statements. Following [121], and references therein, it is easy to see that for $I_n^+(XX)$ we have $f(z) = -(z^n + z^{-n})$ which have $2n$ zeros on the unit circle and so its ground state is critical and in the limit of large L it can be described by a CFT with the central charge $c = n$. This can be also checked by calculating the entanglement entropy analytically (using the FH theorem [92]) and numerically (using the Peschel method [14], see appendix B) by hiring the correlation matrix $C_{jk} = \langle c_j^\dagger c_k\rangle$. For the ground state of infinite size $I_n^+(XX)$ we have [1]

$$C_{jk} = \frac{1}{\pi(j-k)}\sum_{m=1}^{n}(-1)^{m+n}\sin\left(\frac{\pi(2m-1)(j-k)}{2n}\right), \tag{6.13}$$

and $C_{jj} = \frac{1}{2}$. The above $\mathbf{C}$ matrix can be also found as the correlation matrix of one of the excited states with energy zero of the Hamiltonian (6.9). The correlation matrix of the ground state of the infinite size $I_m^-(XX)$ can be also calculated easily and it is [1]

$$C_{jk} = \frac{-i}{2\pi(j-k)}\sum_{n=[-m/2]+1}^{[m/2]}\left(e^{\frac{2in\pi}{m}(j-k)} - e^{i\frac{(2n-1)\pi}{m}(j-k)}\right), \tag{6.14}$$

and $C_{jj} = \frac{1}{2}$. The central charge of the underlying CFT is $c = m$. In the Figure 2 we show the logarithmic behavior (and the corresponding coefficient) of the entanglement entropy of the ground state of $I_m^-(XX)$ for $m = 1, 2, 3$[2]. Based on the above arguments

[1] We note that this sum can be simplified formally but for numerical calculations the above form is more useful

[2] We note that although the two correlation matrices (6.13) and (6.14) are different they have the same set of eigenvalues

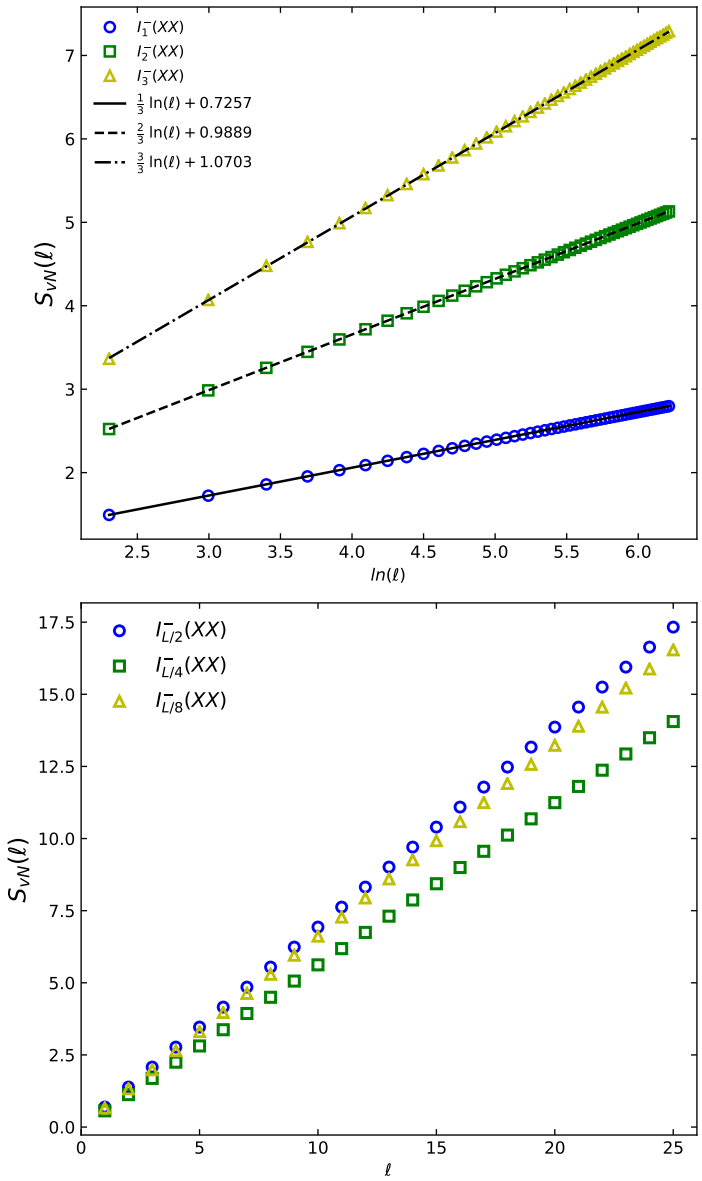


Figure 2 – Top: bipartite von Neumann entropy with respect to the logarithm of the size of the subsystem for the ground state of $I_m^-(XX)$ with $m = 1, 2, 3$. Bottom: bipartite von Neumann entropy with respect to the size of the subsystem for the ground state of $I_m^-(XX)$ with $m = \frac{L}{8}, \frac{L}{4}, \frac{L}{2}$, and $L = 200$

one can conclude that there are infinite conformal excited states with logarithmic scaling of the entanglement in the spectrum of H_{XX} with the central charge $c = m$, where m can be any integer number. In the above, we looked to the finite m when L goes to infinity. However, it is clear that if m is comparable to L, then one would expect for large L probably a volume-law instead of a logarithmic behavior. This is indeed correct as it was shown in the Ref [93] for $I_n^+(XX)$. The entanglement entropy of these excited states follows a volume-law with a subleading term which is logarithmic. In the Figure 2 we show the linear behavior of the entanglement entropy of the ground state of $I_m^-(XX)$ for $m = \frac{L}{8}, \frac{L}{4}, \frac{L}{2}$[2]. In the $L \to \infty$ there are an infinite number of this kind of energy excited states too. It is just enough to take $n = \alpha L$ where $0 < \alpha < 1$. Note that in these cases the

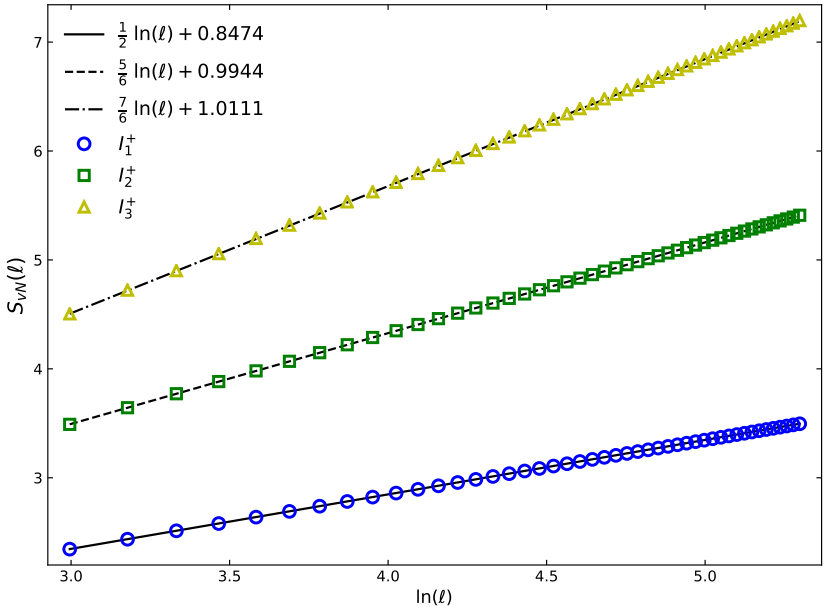


Figure 3 – Bipartite von Neumann entropy with respect to the logarithm of the size of the subsystem for the ground state of I_m^+ with $m = 1, 2, 3$ produced out of the critical Ising parameters.

corresponding Hamiltonians $I_n^+(XX)$ are not local Hamiltonians. We note that there are also excited states that follow an area-law. For example, the states $|11...1\rangle$ and $|00...0\rangle$ have energy zero and trivially follow an area-law. In the case of I_m^- as we will discuss soon this observation is more pronounced.

For generic free fermions, the arguments are similar: the Hamiltonian $H = I_0^+$ commutes with I_m^- which means that the ground state of these integrals of motion should appear in the excited states of H. This means that even if the Hamiltonian is gapped (such as the gapped XY-chain) with the area-law property for the GS, there are still infinite excited states in the spectrum that are conformal invariant with the central charge $c = m$ and follow the logarithmic behavior. Of course, there are also an infinite number of excited states that follow the volume-law too. Interestingly, one can also argue that although the Hamiltonians I_m^- have critical ground states, they also have an infinite number of excited states that follow an area-law. This simply because independent of the parameters in $H = I_0^+$ the Hamiltonians I_m^- commute with it. Clearly, we have infinite possibilities to produce Hamiltonians I_n^+ with gapped ground states that follow an area-law. If one starts with a critical Hamiltonian H with half-integer central charge (for example an Ising critical chain) then it is easy to see that the Hamiltonians I_m^+ will have ground states with all the possible half integer numbers, i.e. $c = n + \frac{1}{2}$. That means, for example, the Hamiltonian of the critical Ising chain has excited states with all the possible integer and half-integer numbers. In the Figure 3 we show the logarithmic behavior (and the corresponding coefficients) of the entanglement entropy of the ground state of the I_n^+, associated to the critical transverse field Ising chain, for $n = 1, 2, 3$.

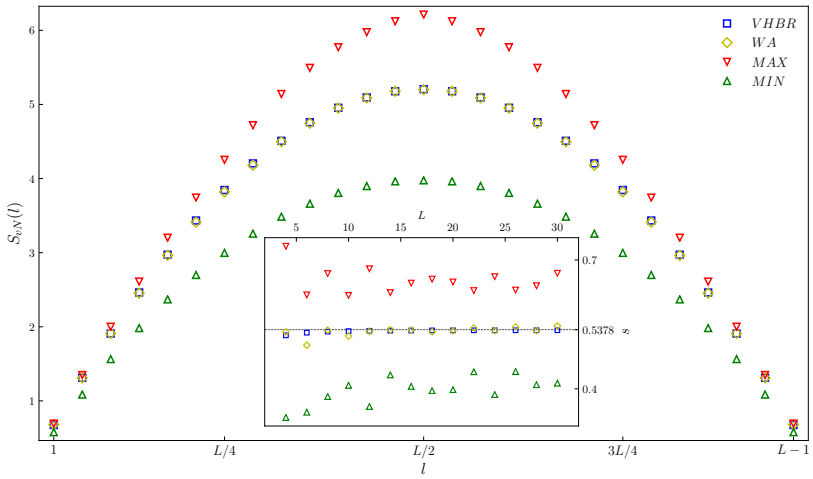


Figure 4 – Various averagings of the entanglement entropy of the eigenstates of free fermions (XX-chain) in a periodic chain with $L = 28$ sites. Results are plotted as a function of the linear subsystem size l. In the inset $s = \frac{S_{vN}(L/2)}{\frac{L}{2}\ln 2}$ is plotted as a function of the system size for $L \leq 30$. As one can see, VHBR (blue square) and WA (yellow diamond) averages converge to the number 0.5378 reported in [102]. However, the MAX (red triangle) and MIN (green triangle) do not converge to the same value.

6.1.1 VHBR averaging and a proposal for measurement

In the case of the periodic free fermions, we expect a lot of degeneracy in the excited states. As it was discussed in more detail in the Appendix C the number of independent energies over the size of the Hilbert space decays exponentially with respect to the size of the system which indicates an enormous number of degeneracies. The way that one defines the excited state might be significant in getting area, logarithmic or volume law for the entanglement entropy. Recently in [102, 106] it was observed that if one takes all the eigenstates produced by the creation operators $\eta_k^\dagger$ as:

$$|\psi\rangle = \Big(\prod_{k_n \in \mathbb{E}} \eta_{k_n}^\dagger\Big)\,|0\rangle\,, \tag{6.15}$$

and calculates the bipartite entanglement entropy of a connected region the result is universal and independent of the Hamiltonian. Here, we would like to comment that the result can be different if one takes into account the degeneracies and different averaging based on the degeneracies.

Averaging Types: Because of the huge degeneracy in the spectrum of periodic free fermions it is clear that one has a lot of freedom in choosing an eigenstate with different amount of entanglement. The more degeneracy means that there is more freedom in picking a state with very large or very small entanglement content. The sum of two maximmaly entangled states can be in principle a product state with zero entanglement. The reverse is also true, the sum of two product states can be maximmaly entangled. When there is a degeneracy in the spectrum it is not feasible to look for a state with max/min entanglement. After creating all the eigenstates, we calculated the entanglement entropy using the Peschel

formula [14] which is valid also for the excited eigenstates. Note that this is not the case for an arbitrary state due to the lack of Wick's theorem. After getting the entanglement entropy for all the eigenstates, we averaged these entanglements for L_A from 1 to $L-1$ in four different ways.

- Averaging over all the entanglement entropies without counting for degeneracies (VHBR mean), as in [102, 106], and averages all the eigenstates without looking at their energies.
- identify and group the degenerate states and average over the entanglement entropy inside each degenerate group, then we average over all the averaged entanglement entropies (WA mean).
- Identifying the degenerate states and group the states with the same energies and group the states with the same energies. Then, finding the minimum value of the entropy in any set of the degenerate eigenstates, and then calculating the average of this minimum entropies (MIN mean).
- Similar to the lase case, finding the maximum value of entropy in any set of degenerate eigenstates, and then calculating the average of this maximum entropies (MAX mean).

In Figure 4, we did the averaging for the XX chain in four different ways above. In Figure 4, one can see that the VHBR and the WA averages converge to the same value but the MIN and the MAX averages converge to the different values. This clearly shows that the averaging done in the [102, 106] is special.

Remarkably, the averaging and universality proposed in these papers have a good chance to be measured experimentally. This is because of a recent duality proposed in [120]. In this work, it was shown that there is a one to one correspondence between bipartite entanglement entropy of the excited states (produced by the $\eta_k^\dagger$) of the XX-chain and the entanglement entropy of one eigenstate (the ground state for the case of $l=\frac{L}{2}$) but with different partition. There are 2^L possible multi interval bipartitions for the eigenstate of the XX-chain which is identically equal to the one interval bipartite entanglement entropy of 2^L excited states. Using this method it is possible to regenerate the universal figure proposed in [102], see Figure 4. Consider the XX-chain Hamiltonian with the eigenstates $|K\rangle$, where $K=\{k_1,k_2,...,k_M\}\subset\{0,...,L-1\}$ are the excited modes. Then consider a subset of sites $A=\{x_1,x_2,...,x_M\}\subset\{0,...,L-1\}$. Based on [120] if we consider $S(A;\psi)$ as the entanglement of the sites A with respect to the rest for the pure state $|\psi\rangle$, then we have

$$S(A;K)=S(K;A), \tag{6.16}$$

for any entropy functional. We now discuss a few examples of the above equality. For the half-filling to get the ground state, we need to fill all the negative modes which make

half of the modes that are adjacent in the set K. This means the entanglement entropy of the ground state for the set A is equal to the entanglement entropy of the half of the system for an eigenstate with the modes A excited. Of course, if one averages over the entanglement entropy of all the possible sets A one recover the average entanglement entropy VHBR for half of the system. Now consider we are interested in the averaging of VHBR for one site, in another word, $A = \{x_1\}$. This can be calculated by finding the average of the entanglement entropy of all the multi interval bipartitions of the state $K = \{k_1\}$ with just one mode excited. The rest of the VHBR graph can be produced similarly by calculating the average of the entanglement entropy of all the multi interval bipartitions of one eigenstate.

The above remarkable observation means that one can calculate the average entanglement entropy by just calculating the entanglement entropy of all the multi interval bipartitions for a single eigenstate. The entanglement entropy of different partitions in the spin chains has been already studied theoretically and experimentally in [122, 123]. The method proposed and implemented in these works gives access to the entanglement entropy of all the 2^L different partitions for a particular state. Extension of this technique to free fermions can make it an outstanding method to measure the universal average entanglement entropy proposed in [102, 106]. It is important to mention that because of the non-local nature of the JW transformation the average over the entanglement of all the possible bipartitions of the GS in the free fermions and the equivalent spin chains are not equal [124].

Conclusions

We showed that independent of the gap a generic translational invariant free-fermion Hamiltonian in one dimension has infinite eigenstates that follow logarithmic-law of entanglement and can be described by CFT. We argued that because of the huge degeneracy, even a Hamiltonian with a critical GS can in principle have a lot of excited states with an area-law behavior. Similar conclusions are valid also for the excited states of the corresponding spin chains. We also proposed a method to measure the recently proposed universal average entanglement entropy over all the exponential number of eigenstates of a generic free fermion Hamiltonian by averaging over multi interval bipartite EE of just a *single* eigenstate of the XX-chain. See [16] for the the same discussion of generic HOs in one dimension. It will be interesting to explore in more detail the averaging over the multi interval bipartite EE of the eigenstates of the generic free fermions and also spin chains.

— 7 —

Entanglement entropy in quantum spin chains with broken parity number symmetry

There exist many quantum spin chains which can be transformed into quadratic fermion models using Jordan Wigner (JW) transformation, the spin-1/2 XY chain is just one example of such spin chains. These fermionic models have been studied thoroughly in the past, and it was shown that they are exactly solvable [24]. In the context of the non-interacting fermions, the calculation of some quantities such as reduced density matrix (RDM) [13, 15], entanglement [65, 67, 68, 69] and formation probabilities [125, 126, 127] can be written in terms of correlation functions, which reduces the adversity of such calculations. The connection to the free fermion models also makes it possible to study the Rényi entanglement entropy for excited eigenstates of free fermions and related spin chains [92, 94, 95, 93, 102, 107, 16, 128, 129].

Most of the above mentioned studies were based on the bulk properties, however, there are also studies regarding the entanglement entropy in systems with boundaries and impurities. In the presence of boundaries analytical and numerical calculations of the entanglement entropy can be more challenging due to the lack of the translational symmetry. The entanglement entropy of a few quantum chains in the presence of the boundaries has been studied with analytical and numerical techniques, see for instance [130, 131, 132, 133, 134, 84, 111, 135]. An interesting consequence of presence of the boundary is the breach of connection between spin chains and quadratic fermion models, specially in subsystem entanglement [124, 135]. An spin chain (containing L spins) with arbitrary boundary magnetic fields can be modeled as: bulk Hamiltonian plus boundary terms,

$$H_{\text{SpinChain}} = H_{\text{bulk}} + H_{\text{boundary}}. \tag{7.1}$$

The H_{boundary} resembles the effect of boundary on far end sites or spins. For instance, a general boundary condition produced by external magnetic fields reads as $H_{\text{boundary}} = \vec{B}_1.\vec{S}_1 + \vec{B}_L.\vec{S}_L$, where $\vec{S}_1$, $\vec{S}_L$ are spin operators at the beginning and end of the chain, and $\vec{B}_L$, $\vec{B}_1$ denote the preferred direction of alignment of boundary magnetic fields. While such a non uniform boundary condition can be physically valid for a spin chain, the fermionization of such a spin chain would end up in a non-physical fermion model. A fermion model which violates the parity symmetry will break the locality. Locality forbids a Hamiltonian that does not commute with fermionic parity symmetry [136, 137, 138]. However, as far as one is concerned with spin model this violation is not a problem.

Some spin models, such as the XXZ chain, with arbitrary direction of boundary magnetic fields (ADBMF) have been already exactly solved by the thermodynamic Bethe ansatz method [139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149, 150, 151]. However, calculation of some quantities such as the entanglement entropy seems out of reach at this moment. In this work we take advantage of a method proposed in [152, 153], see also [154, 155, 156] to transform a generic quantum spin chain; with H_{bulk} that can be mapped to the Hamiltonian of free fermions; with non uniform magnetic field at the

boundaries into a quadratic fermion Hamiltonian. It is done by adding auxiliary spins to the system with coupling to the boundary spins and enlarging the Hilbert space of the original model. Afterward, we would be able to fermionize the spin system via JW transformation and make use of the general formulation of quadratic fermion Hamiltonians to study the quantities of interest. The quadratic (or bi-linear) form of Hamiltonian in fermionic operators is crucial since the Hamiltonian can be diagonalized exactly and the correlation functions can be reduced to the expectation values of pairs of fermionic operators (Wick theorem [50]). To retrieve the eigenstates of original model, we can use particular projection of new model's eigenstates. In [152], the same method was used to study a fermionic model with linear operator terms, which breaks the parity. In this case, the author couples the auxiliary fermions to every other in the system, and gets a quadratic Hamiltonian.

Starting from the enlarged bi-linear fermionic representation of the Hamiltonian, similar to [152, 154, 156], the degeneracy of (at least) two is expected. This degeneracy results in degenerate ground states with opposing parities, which allows us to find a superposition for the ground state with broken parity number. However, for such an eigenstate, we would not be able to use conventional methods to find the RDM, entanglement and so forth. We study the aspects of this state and how it is related to the ground states of the original boundary magnetic field (BMF) Hamiltonian. Also, the comparison of the correlation of this state with those of the parity symmetry states is investigated. Such an investigation enables us to make an ansatz for RDM based on the correlation matrices. This ansatz was first proposed in [156] for a special type of parity broken state and special type of subsystem. Here, we generalize the previous results and provide a proof for consistency of this ansatz. In addition, the RDM has been calculated in different methods. We also show that all of these results can be extended to arbitrary enigenstates of the Hamiltonian (7.1).

Having the RDM in terms of correlation matrices facilitates the calculation of entanglement. For the parity broken state the behavior of entanglement entropy with respect to parity number is intriguing. An interesting observation is that based on the way one breaks the parity of the ground state entanglement can be minimized or unaffected. Besides, we show that with an adjustment to the Peschel method [13, 65, 66, 15, 67], it is possible to get the entanglement of parity broken state in terms of entanglement of parity protected ground states. With these results, we will be able to study the effect of boundary conditions on the entanglement of subsystem, in particular, change in the direction of magnetic field at boundaries on the value of entanglement entropy.

It is worth mentioning that one can treat the enlarged Hamiltonian as a model of interest and study its different properties independent of the quantum spin chain with boundaries. This might be an interesting approach to study a phenomena like spontaneous breaking of parity number symmetry. Having this in mind most of our studies and results

go beyond just the quantum spin chains with ADBMF. We find the correlations, reduced density matrix and entanglement for generic eigenstates of the enlarged Hamiltonian. Quite surprisingly, the general features of the results are quite independent of the bulk Hamiltonian.

The remainder of this chapter is structured as follows: In section 7.1 we first summarize the set up and the main results of this chapter. In section 7.2, we start by general quadratic Hamiltonian that one can derive after the addition of extra sites. We, provide a general discussion on diagonalization of such a system, and the connection to the eigenstates of our original model, the BMF Hamiltonian. In section 7.3, we use the result of diagonalization of quadratic Hamiltonian to find the correlation matrices for the generic eigenstates including the most interesting ones, i.e. states with ± 1 parity and the one with no parity. Section 7.4 contains study of the reduced density matrix (RDM). We first present a general formulation of RDM using Berezin integration of Grassmann variables, followed by the RDM in terms of correlation matrices. We address the RDM not only for typical eigenstates of Hamiltonian, but also eigenstates which break the parity. With the results of former sections, we study the entanglement in section 7.5. Notably, we dig to the behavior of entanglement for a state which defies the parity symmetry. In section 7.6 we give an interesting physical interpretation of the parity-broken state based on three-part system. This gives a simple way to reproduce some of our results in especial cases. Finally, in section 7.7, we look at some interesting examples of systems with no parity symmetry. The first being free fermion model with no bulk term, and the second being the XY-spin chain with arbitrary boundary magnetic fields.

7.1 Set-up

Consider the spin chain Hamiltonian

$$H_{\text{SpinChain}} = H_{\text{bulk}} + \vec{B}_1.\vec{S}_1 + \vec{B}_L.\vec{S}_L, \tag{7.2}$$

where $\vec{S}_1$ and $\vec{S}_L$, are spin operators at the beginning and end of the chain, and $\vec{B}_L$, $\vec{B}_1$ are arbitrary boundary magnetic fields. We consider here bulk Hamiltonians, i.e. H_{bulk}, that can be mapped to quadratic free fermions via Jordan-Wigner (JW) transformation. The above Hamiltonian does not have quadratic form after JW transformation and a priory is not clear that can be solved exactly. However, using the ancillary spins, S_0 and S_{L+1} one can transform the above Hamiltonian to

$$H = H_{\text{bulk}} + B_1^x S_0^x S_1^x + B_1^y S_0^x S_1^y + B_1^z S_1^z + B_L^x S_L^x S_{L+1}^x + B_L^y S_L^y S_{L+1}^x + B_L^z S_L^z \tag{7.3}$$

The above Hamiltonian after JW transformation has a quadratic form and can be solved exactly. The Hamiltonian (7.5) is considered with this goal in mind. The eigenstates and eigenvalues of the original Hamiltonian can be found with proper projections (see section

7.2). The idea of using ancillary sites to solve boundary spin chains is already explored before in [152, 153, 154, 155, 156], however, in this work we solve the problem in its most general form without restricting to a particular Hamiltonian. The eigenstates, eigenvalues and correlation functions are found in the most general cases in sections 7.2 and 7.3.

Interestingly all the eigenstates of the Hamiltonian (7.3) have at least the degeneracy of two due to the presence of a zero mode. In the fermionic language the vacuum, i.e. $|0\rangle_\eta$, and the state with the zero mode excited, i.e. $\eta_0^\dagger |0\rangle_\eta$, are degenerate. This means one can define

$$|\beta\rangle = \frac{1}{\sqrt{1+|\beta|^2}}\Big(|0\rangle_\eta + \beta \eta_0^\dagger |0\rangle_\eta \Big); \tag{7.4}$$

as the most generic ground state of this Hamiltonian[1]. In particular, the ground state of the boundary quantum spin chain can be derived out of the especial cases of $\beta = \pm 1$. Due to its generality in sections 7.2 and 7.3 we study some basic properties of this state such as parity and correlation functions. This state has also an interesting interpretation as three part system which we will explore in section 7.6.

In section 7.4 we give two different forms for the reduced density matrix of the generic $|\beta\rangle$ state. We first find the reduced density matrix in fermionic coherent basis. The presented form can be used to calculate the Rényi entanglement entropy as it was shown in section 7.5. We also think that this form is useful to calculate the formation probabilities in the configuration basis which are although interesting for their own sake, we are not going to explore them in this chapter. The second method is a generalization of the results of [156] for generic eigenstates of the generic Hamiltonians with arbitrary β. It is an extension of a method which is based on making an ansatz for the reduced density matrix and then fix the exact form by matching the correlation functions [14]. Our result for $\beta = \pm 1$ gives also the reduced density matrix of the quantum spin chain with arbitrary boundary magnetic fields. Using the results of this section in section 7.5 we write an exact formula for the entanglement entropy of the $|\beta\rangle$ state which its complexity grows polynomially with the size of the subsystem. As before, this also solves the problem of the calculation of the entanglement entropy of the eigenstates of the Hamiltonian (7.2).

In section 7.6 we show that the $|\beta\rangle$ state has a very interesting property. It can be written like a three-part system which helps to understand the entanglement of the ancillary sites with the rest of the system using this simple interpretation. This property makes studying the Hamiltonian (7.3) and its entanglement content interesting for its own sake independent of the original motivation of solving the quantum spin chain with

[1] Note that the same can be done with all the eigenstates. Our results can be extended for the $|\beta\rangle$ states made of each eigenstates.

arbitrary boundary magnetic fields. This has been the main motivation to start with the fermionic version of the enlarged Hamiltonian in section 7.2.

All of the discussions up to section 7.7 are independent of the Hamiltonian and also valid for arbitrary eigenstates of the Hamiltonians (7.2) and (7.3). In section 7.7 we give two explicit examples. The first one is a slight generalization of the Hamiltonian (7.3) without a bulk term. In the first sight this seems oversimplification but interestingly a lot of entanglement properties of the generic Hamiltonian have similar features which was the main motivation for its presentation. To give a non-trivial example we also study the entanglement entropy in the XY chain. The boundary entropy of this model is already studied in [156], however, here we fill a few holes such as the presentation of the exact extra zero modes present in the Ising chain which their form is essential to calculate the entanglement entropy exactly.

7.2 The Hamiltonian

In this section, we introduce a general bi-linear fermionic Hamiltonian which is related to spin chain Hamiltonians with boundary magnetic field (7.1). We first study the general properties of this model and point out the evident zero mode of the model. In subsection 7.2.3, we tend to present the diagonalization procedure using the standard methods. Later, in subsection 7.2.5, we look into the particular eigenstates of the Hamiltonian which does not respect the parity number symmetry. Finally, subsection 7.2.6 presents a set of selection rules to retrieve the eigenvalues of the boundary magnetic field (BMF) model. Interestingly the structure that unfold is very similar to the ones in [156], see also [154] with a slightly different notation.

7.2.1 General properties

We are going to study the quadratic fermionic Hamiltonian of the form:

$$H = H_0 + H_b \tag{7.5}$$

where

$$H_0 = \sum_{i,j=1}^{L} \left[c_i^\dagger A_{ij} c_j + \tfrac{1}{2} c_i^\dagger B_{ij} c_j^\dagger + \frac{1}{2} c_i B_{ji}^* c_j \right] - \frac{1}{2}\mathrm{tr}(\mathbf{A}^*), \tag{7.6}$$

and

$$H_b = \sum_{j=1}^{L} \left[\alpha_j^0 (c_0 c_j - c_0^\dagger c_j) + \alpha_j^{L+1} (c_j c_{L+1}^\dagger + c_j c_{L+1}) + \text{H. C.} \right]. \tag{7.7}$$

As we mentioned in the introduction, H_b part can be related to the boundary terms. Note that the above Hamiltonian is a bit more general than just the extension of a quantum chain with boundaries because the added extra sites 0 and $L+1$ are coupled to all the

sites. Note also that we are not bounded here to any particular dimension. That means all of the upcoming results, as far as we do not talk about spin chains, are valid in arbitrary dimensions. Here, **A** matrix should be Hermitian and **B** matrix should be anti-symmetric. The Hamiltonian can be written as:

$$\mathbf{H} = \frac{1}{2}\begin{pmatrix} \mathbf{c}^\dagger & \mathbf{c} \end{pmatrix} \mathbf{M} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix}, \tag{7.8}$$

where $\begin{pmatrix} \mathbf{c}^\dagger & \mathbf{c} \end{pmatrix}$ stands for $\begin{pmatrix} c_0^\dagger & \cdots & c_{L+1}^\dagger & c_0 & \cdots & c_{L+1} \end{pmatrix}$. The matrix $\mathbf{M}$ in (7.8) should look like below.

$$\mathbf{M} = \left(\begin{array}{ccccc|ccccc} 0 & -\alpha_1^0 & \cdots & -\alpha_L^0 & 0 & 0 & -\alpha_1^{0*} & \cdots & -\alpha_L^{0*} & 0 \\ -\alpha_1^{0*} & & & & -\alpha_1^{L+1*} & \alpha_1^{0*} & & & & -\alpha_1^{L+1*} \\ \vdots & & \mathbf{A} & & \vdots & \vdots & & \mathbf{B} & & \vdots \\ -\alpha_L^{0*} & & & & -\alpha_L^{L+1*} & \alpha_L^{0*} & & & & -\alpha_L^{L+1*} \\ 0 & -\alpha_1^{L+1} & \cdots & -\alpha_L^{L+1} & 0 & 0 & \alpha_1^{L+1*} & \cdots & \alpha_L^{L+1*} & 0 \\ \hline 0 & \alpha_1^0 & \cdots & \alpha_L^0 & 0 & 0 & \alpha_1^{0*} & \cdots & \alpha_L^{0*} & 0 \\ -\alpha_1^0 & & & & \alpha_1^{L+1} & \alpha_1^0 & & & & \alpha_1^{L+1} \\ \vdots & & -\mathbf{B}^* & & \vdots & \vdots & & -\mathbf{A}^* & & \vdots \\ -\alpha_L^0 & & & & \alpha_L^{L+1} & \alpha_L^0 & & & & \alpha_L^{L+1} \\ 0 & -\alpha_1^{L+1} & \cdots & -\alpha_L^{L+1} & 0 & 0 & \alpha_1^{L+1*} & \cdots & \alpha_L^{L+1*} & 0 \end{array}\right). \tag{7.9}$$

For later use, we define the following spin operators at positions 0 and $L+1$,

$$\sigma_0^x = c_0 + c_0^\dagger \quad \text{and} \quad \sigma_{L+1}^x = (1 - 2c_0c_0^\dagger)\prod_{l=1}^{L}(1 - 2c_l^\dagger c_l)(c_{L+1} + c_{L+1}^\dagger). \tag{7.10}$$

These operators commute with each other and the Hamiltonian (7.5); i.e.

$$\left[H, \sigma_{L+1}^x\right] = [H, \sigma_0^x] = \left[\sigma_0^x, \sigma_{L+1}^x\right] = 0. \tag{7.11}$$

The above relations are important in upcoming sections.

7.2.2 Zero mode eigenstates

The **M** matrix in (7.8) has at least two eigenvectors with zero eigenvalues. These eigenvectors correspond to the modes with zero energy. Later on in this chapter, we present a formulation (section 7.2.3) which simplifies the effort to find the correlations (section 7.3), reduced density matrix (section 7.5) and other properties of the system such as entanglement. To use such a formulation, one needs to identify and write the zero eigenvectors in a correct form (see the following subsection).

Due to the form of the **M** matrix (7.9), we expect to have two zero modes. These zero modes do not depend on the parameters and interactions of the system. They can be

written as:

$$\left|u_0^1\right\rangle = \begin{pmatrix} \sqrt{a}e^{i\theta_1} \\ 0 \\ \vdots \\ 0 \\ \sqrt{\frac{1}{2}-a}e^{i\phi_1} \\ \sqrt{a}e^{i\theta_1} \\ 0 \\ \vdots \\ 0 \\ -\sqrt{\frac{1}{2}-a}e^{i\phi_1} \end{pmatrix}, \qquad \left|u_0^2\right\rangle = \begin{pmatrix} \sqrt{\frac{1}{2}-a}e^{i\theta_2} \\ 0 \\ \vdots \\ 0 \\ -\sqrt{a}e^{i\phi_2} \\ \sqrt{\frac{1}{2}-a}e^{i\theta_2} \\ 0 \\ \vdots \\ 0 \\ \sqrt{a}e^{i\phi_2} \end{pmatrix}. \tag{7.12}$$

The orthogonality condition of these states requires the following equality to hold for the parameters

$$\theta_1 - \theta_2 = \phi_1 - \phi_2. \tag{7.13}$$

The above zero modes are independent of the parameters of the Hamiltonian. In the rest, for the sake of simplicity, we take all the angles $(\theta_1, \theta_2, \phi_1, \phi_2)$ to be zero and put $a = \frac{1}{4}$. Taking other values does not change the upcoming results. Depending on the values of coupling parameters there could arise more zero modes in spectrum of $\mathbf{M}$ matrix[2].

7.2.3 Diagonalization

The diagonalization of general free fermion is well explained in section 2.3, and I will not going through the same calculation again. In this subsection, I just briefly review the diagonalization and find the eigenstates of the Hamiltonian. the Hamiltonian (7.8) can be diagonalized in the following form:

$$\mathbf{H} = \frac{1}{2}\begin{pmatrix} \mathbf{c}^\dagger & \mathbf{c} \end{pmatrix}\mathbf{U}^\dagger\mathbf{U}\mathbf{M}\mathbf{U}^\dagger\mathbf{U}\begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix} = \frac{1}{2}\begin{pmatrix} \eta^\dagger & \eta \end{pmatrix}\begin{pmatrix} \mathbf{\Lambda} & 0 \\ 0 & -\mathbf{\Lambda} \end{pmatrix}\begin{pmatrix} \eta \\ \eta^\dagger \end{pmatrix}; \tag{7.14}$$

The matrix $\mathbf{\Lambda}$ is a diagonal matrix with non-negative entries and matrix $\mathbf{U}$ has the block from:

$$\mathbf{U} = \begin{pmatrix} g & h \\ h^* & g^* \end{pmatrix}. \tag{7.15}$$

The Hamiltonian can also be written with respect to new fermionic operators (Bogoliubov fermions) as

$$\mathbf{H} = \sum_k \lambda_k \eta_k^\dagger \eta_k - \frac{1}{2}\mathrm{tr}(\mathbf{\Lambda}), \quad \text{where} \quad \begin{pmatrix} \boldsymbol{\eta} \\ \boldsymbol{\eta}^\dagger \end{pmatrix} = \mathbf{U}\begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix}. \tag{7.16}$$

[2] See section 7.7.2.

From (2.47) and special form of U matrix, we get the following constrains on the elements of $\mathbf{g}$ and $\mathbf{h}$ matrices:

$$g_{k,L+1} = h_{k,L+1} \quad \text{and} \quad g_{k,0} = -h_{k,0} \quad \text{for} \quad k \neq 0 \tag{7.17}$$

To conclude the diagonalization part, we write the explicit expression of η operators:

$$\eta_k = \sum_{j=0}^{L+1} g_{kj}c_j + h_{kj}c_j^\dagger = g_{k0}(c_0 - c_0^\dagger) + \sum_{j=1}^{L}(g_{kj}c_j + h_{kj}c_j^\dagger) + g_{kL+1}(c_{L+1} + c_{L+1}^\dagger); \quad k \neq 0 \tag{7.18}$$

$$\eta_0 = \frac{1}{2}\Big(c_0 + c_{L+1} + c_0^\dagger - c_{L+1}^\dagger\Big). \tag{7.19}$$

From above, we can also write the c-fermions in terms of η-operators as:

$$c_k = \sum_{j=1}^{L+1}(g_{j,k}^*\eta_j + h_{j,k}\eta_j^\dagger); \quad k \neq 0, L+1, \tag{7.20}$$

$$c_0 = \tfrac{1}{2}\eta_0 + \tfrac{1}{2}\eta_0^\dagger + \sum_{j=1}^{L+1}(g_{j,0}^*\eta_j - g_{j,0}\eta_j^\dagger), \tag{7.21}$$

$$c_{L+1} = \tfrac{1}{2}\eta_0 - \tfrac{1}{2}\eta_0^\dagger + \sum_{j=1}^{L+1}(g_{j,L+1}^*\eta_j + g_{j,L+1}\eta_j^\dagger). \tag{7.22}$$

This final result means that the following commutation (anticommutation) relations hold (for $k \neq 0$)

$$\Big[\sigma_{L+1}^x, \eta_k\Big] = \Big[\sigma_{L+1}^x, \eta_k^\dagger\Big] = 0, \tag{7.23}$$

$$\Big\{\sigma_0^x, \eta_k\Big\} = \Big\{\sigma_0^x, \eta_k^\dagger\Big\} = 0. \tag{7.24}$$

Anticommutations (7.24) will be useful in subsection 7.2.6 for sectorization of eigenstates of the Hamiltonian (7.5).

7.2.4 Eigenstates in configuration basis

As it was explained in section 2.3.3, the vacuum state $|0\rangle_\eta$ is the state which is annihilated by the action of all η_k operators,

$$\eta_k |0\rangle_\eta = 0, \quad \forall\, k. \tag{7.25}$$

One can write the $|0\rangle_\eta$ as a superposition of configurations of the c-fermions [13]. It is called the configurational basis of such a state. For even size, if the parity of $|0\rangle_\eta$ is $+1$ then we have:

$$|0\rangle_\eta = \Big(\det[\mathbf{I} + \mathbf{R}^\dagger\mathbf{R}]\Big)^{-\frac{1}{4}} e^{\frac{1}{2}\sum_{i,j} R_{ij}c_i^\dagger c_j^\dagger} |0\rangle_c \tag{7.26}$$

where $c_j |0\rangle_c = 0$ for all j, and the $\mathbf{R}$ matrix is an antisymmetric matrix defined as $\mathbf{g}.\mathbf{R} + \mathbf{h} = 0$. The (7.26) works only for the case where parity of the $|0\rangle_\eta$ is $+1$, and/or the matrix $\mathbf{g}$ is invertible. Otherwise, to use the above equation, one needs to do a canonical

transformation to change the parity of the vacuum for η-fermions, and/or to make the $\mathbf{g}$ invertible [53]. For more details see also section 2.3.3.

As a matter of fact, any eigenstate of Hamiltonian (7.5) (with parity $+1$) can be written in configurational basis in an exponential form. Excited states are created by exciting different modes on the vacuum (7.25) as:

$$|\psi\rangle = |k_1, k_2, \cdots, k_N\rangle = \prod_{k_j \in \mathbb{E}} \eta^\dagger_{k_j} |0\rangle\,; \qquad E_\psi = \sum_{k_j \in \mathbb{E}} \lambda_{k_j} - \frac{1}{2}\mathrm{tr}(\mathbf{\Lambda}), \tag{7.27}$$

where the set $\mathbb{E}$ can be any subset of indices from 0 to $L+1$. We denote the set of indices of excited modes as $\mathbb{E}$ and the set of indices which are not excited as $\bar{\mathbb{E}}$ ($\bar{\mathbb{E}} \cup \mathbb{E} = \{0, 1, \cdots, L+1\}$). Assume that we can write the following excited state in the configurational form as:

$$|\psi\rangle = C^\psi e^{\frac{1}{2}\sum_{i,j} R^\psi_{ij} c^\dagger_i c^\dagger_j} |0\rangle_c\,, \tag{7.28}$$

where $C^\psi = (\det[\mathbf{I} + \mathbf{R}^{\psi\dagger}\mathbf{R}^\psi])^{-\frac{1}{4}}$. For this excited state we have: The generalized formula for the $\boldsymbol{R}^\psi$ would be:

$$\mathfrak{g}\boldsymbol{R}^\psi + \mathfrak{h} = 0, \tag{7.29}$$

where $\mathfrak{g}$ and $\mathfrak{h}$ are generalized versions of $\mathbf{g}$ and $\mathbf{h}$ given by

$$\mathfrak{g}_{nm} = \begin{cases} g_{nm} & if\ n \in \bar{\mathbb{E}} \\ h^*_{nm} & if\ n \in \mathbb{E} \end{cases} \qquad \mathfrak{h}_{nm} = \begin{cases} h_{nm} & if\ n \in \bar{\mathbb{E}} \\ g^*_{nm} & if\ n \in \mathbb{E} \end{cases} \tag{7.30}$$

Note that one should check for the necessary conditions to be able to use relation above for excited states. For more details please look at secton 2.3.4. The (7.28) gives an excited eigenstate in the configuration basis which is advantageous in the study of entanglement in later sections.

7.2.5 Parity broken state

The quadratic Hamiltonian (7.5) commutes with the parity operator defined as $\mathbf{P} = (-1)^{\hat{N}}$ where $\hat{N} = \sum_{l=0}^{L+1} c^\dagger_l c_l$ is the fermion number operator. This means that the eigenstates of the Hamiltonian have fixed parity $P = \pm 1$. One can have eigenstates that do not respect the parity and these types of states are very interesting to study. For instance, these types of states are related to the ground state of spin systems with boundary magnetic fields which one example is given in section 7.7.2.

We define a parity broken state (β-defected parity state) as:

$$|\beta\rangle = \frac{1}{\sqrt{1+|\beta|^2}}\Big(|0\rangle_\eta + \beta\eta^\dagger_0 |0\rangle_\eta\Big); \tag{7.31}$$

where β can be a complex number. The expectation value of parity for such a state is given by

$$P(\beta) = \langle\beta|\,\mathbf{P}\,|\beta\rangle = \begin{cases} \frac{|\beta|^2-1}{|\beta|^2+1} & P_0 = -1, \\ \\ \frac{1-|\beta|^2}{1+|\beta|^2} & P_0 = +1, \end{cases} \tag{7.32}$$

where P_0 is the parity of vacuum state. The first excited state after the vacuum is created by $\eta_0^\dagger\,|0\rangle$ which inevitably has the same energy as the vacuum, while this excited state has parity -P_0. In fact β can be considered as a parameter which can be tuned to break the parity.

We define the state $|G_\pm\rangle$ by taking $\beta = \pm 1$ as:

$$|G_\pm\rangle = \frac{1}{\sqrt{2}}\Big(\,|0\rangle_\eta \pm \eta_0^\dagger\,|0\rangle_\eta\,\Big). \tag{7.33}$$

These states are especial cases of β-broken parity states and have interesting properties which cares for special attention. As an example, these states are related to the ground state of Hamiltonian with boundary magnetic field (see page 82). Other useful properties of these two states are

$$\sigma_0^x\,|G_\pm\rangle = \pm\,|G_\pm\rangle \quad \text{and} \quad \sigma_{L+1}^x\,|G_\pm\rangle = \delta_\pm\,|G_\pm\rangle\,. \tag{7.34}$$

The $\delta_\pm = \pm$ can be calculated with respect to the expectation values of Majorana fermions [156]. For instance, one can write:

$$\delta_+ = (i)^{L+1}\mathrm{Pf}[\boldsymbol{\mathcal{D}}], \tag{7.35}$$

where

$$\boldsymbol{\mathcal{D}} = \begin{pmatrix} 0 & \langle\bar\gamma_0\gamma_1\rangle & \langle\bar\gamma_0\bar\gamma_1\rangle & \cdots & \langle\bar\gamma_0\gamma_{L+1}\rangle \\ \langle\gamma_1\bar\gamma_0\rangle & 0 & \langle\gamma_1\bar\gamma_1\rangle & \cdots & \langle\gamma_1\gamma_{L+1}\rangle \\ \langle\bar\gamma_1\bar\gamma_0\rangle & \langle\bar\gamma_1\gamma_1\rangle & 0 & \cdots & \langle\bar\gamma_1\gamma_{L+1}\rangle \\ \vdots & \vdots & \vdots & & \vdots \\ \langle\gamma_{L+1}\bar\gamma_0\rangle & \langle\gamma_{L+1}\gamma_1\rangle & \langle\gamma_{L+1}\bar\gamma_1\rangle & \cdots & 0 \end{pmatrix}. \tag{7.36}$$

in above, $\mathrm{Pf}[\boldsymbol{\mathcal{D}}]$ is the Pfaffian of the matrix $\mathcal{D}$, and Majorana fermions are defined as $\gamma_j = c_j^\dagger + c_j$ and $\bar\gamma_j = i(c_j^\dagger - c_j)$. In (7.36), the $\langle\cdots\rangle$ stands for the expectation value with respect to the vacuum state of the η-operators ($|0\rangle$).

7.2.6 Eigenstates of boundary magnetic field model

Since the eigenstates of boundary magnetic field model is related to those of Hamiltonian (7.5), we are going to present selection rules to get the desired eigenstates. In fact, Hilbert space of Hamiltonian (7.5) is 4 times bigger than BMF Hamiltonian.

The Hilbert space of Hamiltonian (7.5) can be divided into 4 sub-spaces. Each sub-space can be identified using eigenvalues of operators σ_0^x and σ_{L+1}^x acting on states $|G_\pm\rangle$. We can make the following argument: consider $\delta_+ = 1$, which means $|G_+\rangle$ belongs to the sector marked by the pair $(\langle G_\pm|\,\sigma_0^x\,|G_\pm\rangle\,, \langle G_\pm|\,\sigma_{L+1}^x\,|G_\pm\rangle)$. Then due to commutation (anticommutation) relations (7.23) and (7.24) all the states

$$\prod_{j=1}^{n} \eta_{k_j}^\dagger\,|G_+\rangle\,, \qquad n \text{ is even.} \tag{7.37}$$

also belong to $(+,+)$. Note that in the above expression $0 < k_j < k_{j+1} < L+1$ which means that the dimension of $(+,+)$ sub-space is 2^L. Next, in this case ($\delta_+ = +1$), the state $|G_-\rangle$ and the following states belong to $(-,-)$ sector,

$$\prod_{j=1}^{n} \eta_{k_j}^\dagger\,|G_-\rangle\,, \qquad n \text{ is even.} \tag{7.38}$$

For the two other sectors we have:

$$\begin{aligned} &\prod_{j=1}^{n} \eta_{k_j}^\dagger\,|G_+\rangle\,, \qquad n \text{ is odd.} \qquad (-,+),\\ &\prod_{j=1}^{n} \eta_{k_j}^\dagger\,|G_-\rangle\,, \qquad n \text{ is odd.} \qquad (+,-), \end{aligned} \tag{7.39}$$

In the case of $\delta_+ = -1$, we have the following eigenstates for each sector,

$$\prod_{j=0}^{n} \eta_{k_j}^\dagger\,|G_+\rangle\,, \qquad n \text{ is even,} \qquad (+,-), \tag{7.40}$$

$$\prod_{j=0}^{n} \eta_{k_j}^\dagger\,|G_-\rangle\,, \qquad n \text{ is even,} \qquad (-,+), \tag{7.41}$$

$$\prod_{j=1}^{n} \eta_{k_j}^\dagger\,|G_+\rangle\,, \qquad n \text{ is odd,} \qquad (-,-), \tag{7.42}$$

$$\prod_{j=1}^{n} \eta_{k_j}^\dagger\,|G_-\rangle\,, \qquad n \text{ is odd,} \qquad (+,+). \tag{7.43}$$

As an example in the $(+,+)$ sector, we can write:

$$|\phi_k\rangle = |+\rangle_0 \otimes |\varphi_k\rangle \otimes |+\rangle_{L+1}\,, \tag{7.44}$$

where $|\phi_k\rangle$ is an eigenstate of Hamiltonian (7.5), $|+\rangle_{0,L+1}$ are eigenstates of σ^x at the position 0 and $L+1$. The $|\varphi_k\rangle$ is an eigenstate of the BMF model. Knowing $|\phi_k\rangle$, we can obtain the $|\varphi_k\rangle$.

The above argument means that to know the sector $(+,+)$ we need to figure out the value of δ_+. The ground state of the Hamiltonian with boundary magnetic field is going to be one of the following two states:

$$|G_+\rangle \qquad \delta_+ = +1, \tag{7.45}$$

$$\eta_{min}^\dagger\,|G_-\rangle \qquad \delta_+ = -1. \tag{7.46}$$

In above, $\eta^{\dagger}_{min}$ creates the mode with smallest non-zero energy.

It is interesting to mention that exist transformations which change the sign of boundary couplings in the Hamiltonian (7.5). Such transformations could be $T_{b_L} = \sigma^z_{L+1}$ and $T_{b_1} = \sigma^z_0$ where they change the sign of x and y component of boundary couplings ($\overrightarrow{b}_1$, $\overrightarrow{b}_L$ or equivalently α^0_1, α^{L+1}_L), without affecting the energy spectrum of the Hamiltonian:

$$T^{\dagger}_{b_1} T^{\dagger}_{b_L} H(b_{1,x}, b_{1,y}, b_{1,z}, b_{L,x}, b_{L,y}, b_{L,z}) T_{b_L} T_{b_1} = H(-b_{1,x}, -b_{1,y}, b_{1,z}, -b_{L,x}, -b_{L,y}, b_{L,z}). \quad (7.47)$$

As a consequence, if the eigenstates of the BMF Hamiltonian (7.1) is found in one of the sectors of the Hilbert space of the Hamiltonian (7.5), then other sectors are related to the eigenstates of BMF Hamiltonians with different signs of boundary couplings. For example, if a typical eigenstate of the BMF Hamiltonian like $|\varphi_k\rangle$, is in the $(+,+)$ sector, then from (7.44) we have $|+\rangle_0 \otimes |\varphi_k\rangle \otimes |+\rangle_{L+1}$ for the eigenstates of Hamiltonian (7.5). The action of $T_{b_1} T_{b_L}$ on a state like $|\phi_k\rangle$ would be

$$T_{b_1} T_{b_L} |\phi_k\rangle = |-\rangle_0 \otimes |\varphi_k\rangle \otimes |-\rangle_{L+1}, \quad (7.48)$$

which is equal to changing the sign of boundary couplings. Therefore, $|\varphi_k\rangle$ would be an eigenstate of BMF Hamiltonian with boundary couplings: $-b_{1,x}$, $-b_{1,y}$, $-b_{L,x}$ and $-b_{L,y}$. Equivalently, spectrum of of BMFH with negative couplings at boundary can be found in the $(-,-)$ sector of Hamiltonian (7.5).

7.3 Correlation functions

In this section, we would like to calculate the correlation matrix for different eigenstates of the system. It is more convenient to calculate the correlation matrices for Majorana fermions. For instance, one can use Majorana fermion correlations to calculate the entanglement in the system (for particular eigenstates). We introduce Majorana fermions as $\gamma_i = c_i + c^{\dagger}_i$ and $\bar{\gamma}_i = i(c^{\dagger}_i - c_i)$. We symbolize the correlation matrices as:

$$\langle \bar{\gamma}_j \gamma_k \rangle = iG_{jk}, \qquad \langle \gamma_j \gamma_k \rangle = K_{jk}, \qquad \langle \bar{\gamma}_j \bar{\gamma}_k \rangle = \bar{K}_{jk}. \quad (7.49)$$

It is useful to write the later two point correlation in a block matrix form denoted by $\mathbf{\Gamma}$ as:

$$\mathbf{\Gamma} = \begin{pmatrix} \boldsymbol{K} - \mathbf{I} & -i\boldsymbol{G}^T \\ i\boldsymbol{G} & \bar{\boldsymbol{K}} - \mathbf{I} \end{pmatrix}. \quad (7.50)$$

One can easily find all the different elements of the $\mathbf{\Gamma}$ matrix. It is possible to write $\mathbf{G}$, $\mathbf{K}$ and $\bar{\mathbf{K}}$ in terms of correlation matrices of c-fermions

$$\begin{aligned} \mathbf{K} &= \mathbf{F}^{\dagger} + \mathbf{F} + \mathbf{C} - \mathbf{C}^T + \mathbb{I}, \\ \bar{\mathbf{K}} &= -\mathbf{F}^{\dagger} - \mathbf{F} + \mathbf{C} - \mathbf{C}^T + \mathbb{I}, \\ \mathbf{G} &= -\mathbf{F}^{\dagger} + \mathbf{F} + \mathbf{C} + \mathbf{C}^T - \mathbb{I}, \end{aligned} \quad (7.51)$$

where $C_{ij} = \langle c_i^\dagger c_j \rangle$ and $F_{ij} = \langle c_i^\dagger c_j^\dagger \rangle$. The $\mathbf{C}$ is a Hermitian matrix and $\mathbf{F}$ is antisymmetric. Therefore, $\mathbf{K}$ and $\bar{\mathbf{K}}$ are Hermitian, and we can conclude that $\mathbf{G}$ is real. Knowing these properties, we can prove that the $\mathbf{\Gamma}$ correlation matrix is Hermitian too. All the analysis so far are valid for arbitrary eigenstates of the Hamiltonian (7.5). In the rest, the correlations for vacuum and zero mode excited eigenstate (ZME state or $\eta_0^\dagger |0\rangle_\eta$) will be presented in details. The calculation of correlations of excited quasi-particle eigenstates is presented in appendix D.

7.3.1 Correlations for vacuum state

Using the notation introduced in (7.14), we calculate the correlations for the vacuum of η's. In this case, we can write $\mathbf{C}^0 = \mathbf{h}^\dagger.\mathbf{h}$ and $\mathbf{F}^0 = \mathbf{h}^\dagger.\mathbf{g}$, where superscript zero stands for the expectation values calculated in the vacuum state. Putting these relations in (7.51), we get

$$\begin{aligned} \mathbf{K}^0 &= (\mathbf{h}^\dagger + \mathbf{g}^\dagger).(\mathbf{h} + \mathbf{g}), \\ \bar{\mathbf{K}}^0 &= (\mathbf{h}^\dagger - \mathbf{g}^\dagger).(\mathbf{h} - \mathbf{g}), \\ \mathbf{G}^0 &= (\mathbf{h}^\dagger - \mathbf{g}^\dagger).(\mathbf{h} + \mathbf{g}). \end{aligned} \tag{7.52}$$

Therefore, for the vacuum of η-operators, we can find the correlations in terms of the elements of $\mathbf{U}$ matrix, which means correlation matrix calculations are straightforward. The above-mentioned correlation matrices have the form $(i, j \neq 0, L+1)$:

$$\mathbf{C}^0 = \left(\begin{array}{c|c|c} \frac{1}{2} & -\sum_{k=1}^{k=L+1} g_{k,0}^* h_{k,j} & \frac{-1}{4} - \sum_{k=1}^{k=L+1} g_{k,0}^* g_{k,L+1} \\ \hline -\sum_{k=1}^{k=L+1} h_{k,j}^* g_{k,0} & (\mathbf{h}^\dagger.\mathbf{h})_{i,j} & \sum_{k=1}^{k=L+1} h_{k,j}^* g_{k,L+1} \\ \hline \frac{-1}{4} - \sum_{k=1}^{k=L+1} g_{k,L+1}^* g_{k,0} & \sum_{k=1}^{k=L+1} g_{k,L+1}^* h_{k,j} & \frac{1}{2} \end{array}\right) \tag{7.53}$$

$$\mathbf{F}^0 = \left(\begin{array}{c|c|c} 0 & -\sum_{k=1}^{k=L+1} g_{k,0}^* g_{k,j} & \frac{1}{4} - \sum_{k=1}^{k=L+1} g_{k,0}^* g_{k,L+1} \\ \hline \sum_{k=1}^{k=L+1} g_{k,j} g_{k,0}^* & (\mathbf{h}^\dagger.\mathbf{g})_{i,j} & -\sum_{k=1}^{k=L+1} g_{k,j} g_{k,L+1}^* \\ \hline -\frac{1}{4} + \sum_{k=1}^{k=L+1} g_{k,L+1}^* g_{k,0} & \sum_{k=1}^{k=L+1} g_{k,L+1}^* g_{k,j} & 0 \end{array}\right) \tag{7.54}$$

Using the relation (7.51), for the correlation of Majorana fermions, we can write:

$$\mathbf{K}^{0} = \left(\begin{array}{c|c|c} 1 & 0 & 0 \\ \hline 0 & (\mathbf{h}^{\dagger}+\mathbf{g}^{\dagger}).(\mathbf{h}+\mathbf{g})_{i,j} & 2\sum_{k=1}^{k=L+1}(h^{*}_{k,j}+g^{*}_{k,j})g_{k,L+1} \\ \hline 0 & 2\sum_{k=1}^{k=L+1} g^{*}_{k,L+1}(h_{k,j}+g_{k,j}) & 1 \end{array}\right), \tag{7.55}$$

$$\bar{\mathbf{K}}^{0} = \left(\begin{array}{c|c|c} 1 & -2\sum_{k=1}^{k=L+1} g^{*}_{k,0}(h_{k,j}-g_{k,j}) & 0 \\ \hline -2\sum_{k=1}^{k=L+1}(h^{*}_{k,j}-g^{*}_{k,j})g_{k,0} & (\mathbf{h}^{\dagger}-\mathbf{g}^{\dagger}).(\mathbf{h}-\mathbf{g})_{i,j} & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \tag{7.56}$$

$$\mathbf{G}^{0} = \left(\begin{array}{c|c|c} 0 & -2\sum_{k=1}^{k=L+1} g^{*}_{k,0}(h_{k,j}+g_{k,j}) & -4\sum_{k=1}^{k=L+1} g^{*}_{k,0}g_{k,L+1} \\ \hline 0 & (\mathbf{h}^{\dagger}-\mathbf{g}^{\dagger}).(\mathbf{h}+\mathbf{g})_{i,j} & 2\sum_{k=1}^{k=L+1}(h^{*}_{k,j}-g^{*}_{k,j})g_{k,L+1} \\ \hline -1 & 0 & 0 \end{array}\right) \tag{7.57}$$

To calculate the higher point correlation functions, one can use the Wick theorem, which is computationally favorable.

7.3.2 Correlations for ZME state

From now on (for the sake of simplicity), we are going to indicate the ZME state by $|\emptyset\rangle = \eta_0^{\dagger}|0\rangle$. This state is degenerate with the vacuum, which is crucial for later studies. For this eigenstate, we get $(i,j \neq 0, L+1)$:

$$\mathbf{C}^{\emptyset} = \begin{pmatrix} \frac{1}{2} & -\sum_{k=1}^{k=L+1} g^{*}_{k,0}h_{k,j} & \frac{1}{4}-\sum_{k=1}^{k=L+1} g^{*}_{k,0}g_{k,L+1} \\ -\sum_{k=1}^{k=L+1} h^{*}_{k,j}g_{k,0} & (\mathbf{h}^{\dagger}.\mathbf{h})_{i,j} & \sum_{k=1}^{k=L+1} h^{*}_{k,j}g_{k,L+1} \\ \frac{1}{4}-\sum_{k=1}^{k=L+1} g^{*}_{k,L+1}g_{k,0} & \sum_{k=1}^{k=L+1} g^{*}_{k,L+1}h_{k,j} & \frac{1}{2} \end{pmatrix} \tag{7.58}$$

$$\mathbf{F}^{\emptyset} = \begin{pmatrix} 0 & -\sum_{k=1}^{k=L+1} g^*_{k,0} g_{k,j} & \frac{-1}{4} - \sum_{k=1}^{k=L+1} g^*_{k,0} g_{k,L+1} \\ \sum_{k=1}^{k=L+1} g_{k,j} g^*_{k,0} & (\mathbf{h}^\dagger.\mathbf{g})_{i,j} & -\sum_{k=1}^{k=L+1} g_{k,j} g^*_{k,L+1} \\ \frac{1}{4} + \sum_{k=1}^{k=L+1} g^*_{k,L+1} g_{k,0} & \sum_{k=1}^{k=L+1} g^*_{k,L+1} g_{k,j} & 0 \end{pmatrix}. \tag{7.59}$$

As a result, the correlation matrices $\mathbf{C}$ and $\mathbf{F}$ are only different in only two elements from state $|0\rangle$ to the state $|\emptyset\rangle$. It can be observed that the correlation matrices $\mathbf{K}$, $\bar{\mathbf{K}}$ does not change from state $|0\rangle$ to $|\emptyset\rangle$. Form of the Majorana correlation matrices are presented below as:

$$\mathbf{K}^{\emptyset} = \mathbf{K}^{0}, \qquad \bar{\mathbf{K}}^{\emptyset} = \bar{\mathbf{K}}^{0}, \tag{7.60}$$

$$\mathbf{G}^{\emptyset} = \begin{pmatrix} 0 & -2\sum_{k=1}^{k=L+1} g^*_{k,0}(h_{k,j} + g_{k,j}) & -4\sum_{k=1}^{k=L+1} g^*_{k,0} g_{k,L+1} \\ 0 & (\mathbf{h}^\dagger - \mathbf{g}^\dagger).(\mathbf{h} + \mathbf{g})_{i,j} & 2\sum_{k=1}^{k=L+1}(h^*_{k,j} - g^*_{k,j}) g_{k,L+1} \\ 1 & 0 & 0 \end{pmatrix}. \tag{7.61}$$

Similar to the result of previous subsection, for higher point functions, one make use of the Wick theorem to calculate the quantity of interest.

7.3.3 Correlations for the general parity broken state

In this subsection we study the correlation function of general states that break the parity, such as $|\beta\rangle$ defined in (7.31). Calculating correlations (or any expectation value) with respect to the state $|\beta\rangle$, is not as trivial as the calculations for eigenstates, since we are not able to use the Wick theorem. However, there could be many subtleties when we come across quantities which are evaluated with respect to $|\beta\rangle$.

For instance, such a subtlety could be calculation of one point function with respect to the $|\beta\rangle$:

$$\langle\beta| c_j |\beta\rangle = \frac{\mathrm{Re}[\beta]}{1+|\beta|^2}\delta_{j,0} + \frac{i\mathrm{Im}[\beta]}{1+|\beta|^2}\delta_{j,L+1} \tag{7.62}$$

The above means that one point correlation functions are not necessarily zero for the state $|\beta\rangle$. In general, we can say that $\langle\beta| \hat{\mathcal{O}} |\beta\rangle$ is not necessarily zero, if operator $\hat{\mathcal{O}}$ has odd number of fermionic operators. Nonetheless, if $\hat{\mathcal{O}}$ does not depend on c_0, $c_0^\dagger$, c_{L+1} and $c_{L+1}^\dagger$ then we can write $\langle\beta| \hat{\mathcal{O}} |\beta\rangle = \langle 0| \hat{\mathcal{O}} |0\rangle$. With this condition, we can assume that the

state $|\beta\rangle$ obeys the Wick theorem. In the following, we denote the correlation matrices by superscript β for the state $|\beta\rangle$. These correlations have the form:

$$\mathbf{C}^{\beta} = \left(\begin{array}{c|c|c} \frac{1}{2} & -\sum_{k=1}^{k=L+1} g^*_{k,0}h_{k,j} & \frac{-1}{4}\frac{1-|\beta|^2}{1+|\beta|^2} - \sum_{k=1}^{k=L+1} g^*_{k,0}g_{k,L+1} \\ \hline -\sum_{k=1}^{k=L+1} h^*_{k,j}g_{k,0} & (\mathbf{h}^{\dagger}.\mathbf{h})_{i,j} & \sum_{k=1}^{k=L+1} h^*_{k,j}g_{k,L+1} \\ \hline \frac{-1}{4}\frac{1-|\beta|^2}{1+|\beta|^2} - \sum_{k=1}^{k=L+1} g^*_{k,L+1}g_{k,0} & \sum_{k=1}^{k=L+1} g^*_{k,L+1}h_{k,j} & \frac{1}{2} \end{array}\right) \tag{7.63}$$

$$\mathbf{F}^{\beta} = \left(\begin{array}{c|c|c} 0 & -\sum_{k=1}^{k=L+1} g^*_{k,0}g_{k,j} & \frac{1}{4}\frac{1-|\beta|^2}{1+|\beta|^2} - \sum_{k=1}^{k=L+1} g^*_{k,0}g_{k,L+1} \\ \hline \sum_{k=1}^{k=L+1} g_{k,j}g^*_{k,0} & (\mathbf{h}^{\dagger}.\mathbf{g})_{i,j} & -\sum_{k=1}^{k=L+1} g_{k,j}g^*_{k,L+1} \\ \hline -\frac{1}{4}\frac{1-|\beta|^2}{1+|\beta|^2} + \sum_{k=1}^{k=L+1} g^*_{k,L+1}g_{k,0} & \sum_{k=1}^{k=L+1} g^*_{k,L+1}g_{k,j} & 0 \end{array}\right) \tag{7.64}$$

Based on the above calculations, the correlations for $|\beta\rangle$ can be written in terms of correlations of vacuum and ZME state. For rest of the correlation matrices, we have:

$$\mathbf{K}^{\beta} = \mathbf{K}^{0}, \qquad \bar{\mathbf{K}}^{\beta} = \bar{\mathbf{K}}^{0}, \tag{7.65}$$

$$\mathbf{G}^{\beta} = \left(\begin{array}{c|c|c} 0 & -2\sum_{k=1}^{k=L+1} g^*_{k,0}(h_{k,j}+g_{k,j}) & -4\sum_{k=1}^{k=L+1} g^*_{k,0}g_{k,L+1} \\ \hline 0 & (\mathbf{h}^{\dagger}-\mathbf{g}^{\dagger}).(\mathbf{h}+\mathbf{g})_{i,j} & 2\sum_{k=1}^{k=L+1}(h^*_{k,j}-g^*_{k,j})g_{k,L+1} \\ \hline \frac{1-|\beta|^2}{1+|\beta|^2} & 0 & 0 \end{array}\right). \tag{7.66}$$

For a higher point correlation like $\hat{\mathcal{O}}$, when operator $\hat{\mathcal{O}}$ contains fermionic creation and annihilation operators at position 0 or $L+1$, then the relation between $\langle\hat{\mathcal{O}}\rangle_0$ and $\langle\hat{\mathcal{O}}\rangle_\beta$ would not be trivial. For example, in some cases, one can have Wick theorem for the $|\beta\rangle$ too. Some of the interesting cases are listed in table 1.

Results of this part can be extended to the zero parity state. Form of the correlation matrices for the state $|G_{\pm}\rangle$ (7.33), can simply be obtained by putting $\beta \to \pm 1$.

Tabela 1 – Terms “even"and “odd"mean that the operator $\hat{\mathcal{O}}$ contains even or odd products of c-operators. Also, $k, l \neq 0, L+1$ and the Einstein summation rule is assumed. The notation $\langle \cdots \rangle_0$ stands for the expectation value calculated in the vacuum state.

	$\hat{\mathcal{O}}$ has no $c_0^{(\dagger)}$ and $c_{L+1}^{(\dagger)}$	
	even	odd
$\langle\beta\vert\, c_0\hat{\mathcal{O}}\,\vert\beta\rangle$	$\frac{\mathrm{Re}[\beta]}{1+\vert\beta\vert^2}\langle\hat{\mathcal{O}}\rangle_0$	$g^*_{k,0}\,\langle 0\vert\,\eta_k\hat{\mathcal{O}}\,\vert 0\rangle$
$\langle\beta\vert\, c_0^\dagger\hat{\mathcal{O}}\,\vert\beta\rangle$	$\frac{\mathrm{Re}[\beta]}{1+\vert\beta\vert^2}\langle\hat{\mathcal{O}}\rangle_0$	$-g^*_{l,0}\,\langle 0\vert\,\eta_l\hat{\mathcal{O}}\,\vert 0\rangle$
$\langle\beta\vert\, c_{L+1}\hat{\mathcal{O}}\,\vert\beta\rangle$	$\frac{i\mathrm{Im}[\beta]}{1+\vert\beta\vert^2}\langle\hat{\mathcal{O}}\rangle_0$	$g^*_{k,L+1}\,\langle 0\vert\,\eta_k\hat{\mathcal{O}}\,\vert 0\rangle$
$\langle\beta\vert\, c_{L+1}^\dagger\hat{\mathcal{O}}\,\vert\beta\rangle$	$\frac{-i\mathrm{Im}[\beta]}{1+\vert\beta\vert^2}\langle\hat{\mathcal{O}}\rangle_0$	$g^*_{l,L+1}\,\langle 0\vert\,\eta_l\hat{\mathcal{O}}\,\vert 0\rangle$
$\langle\beta\vert\, c_0^\dagger c_0\hat{\mathcal{O}}\,\vert\beta\rangle$	$\frac{1}{2}\langle\hat{\mathcal{O}}\rangle_0$	$\frac{2\mathrm{Re}[\beta]}{1+\vert\beta\vert^2}\langle(g^*_{l,0}\eta_l - g_{l,0}\eta_l^\dagger)\hat{\mathcal{O}}\rangle_0$
$\langle\beta\vert\, c_{L+1}^\dagger c_{L+1}\hat{\mathcal{O}}\,\vert\beta\rangle$	$\frac{1}{2}\,\langle 0\vert\,\hat{\mathcal{O}}\,\vert 0\rangle$	$\frac{-2i\mathrm{Im}[\beta]}{1+\vert\beta\vert^2}\langle(g^*_{l,L+1}\eta_l + g_{l,L+1}\eta_l^\dagger)\hat{\mathcal{O}}\rangle_0$
$\langle\beta\vert\, c_0^\dagger c_{L+1}\hat{\mathcal{O}}\,\vert\beta\rangle$	$\frac{1}{4}\frac{\vert\beta\vert^2-1}{\vert\beta\vert^2+1}\langle\hat{\mathcal{O}}\rangle_0 - g^*_{l,0}g_{k,L+1}\langle\eta_l\eta_k^\dagger\hat{\mathcal{O}}\rangle_0$	$\frac{\mathrm{Re}[\beta]}{1+\vert\beta\vert^2}\langle g^*_{l,L+1}\eta_l\hat{\mathcal{O}}\rangle_0 + \frac{i\mathrm{Im}[\beta]}{1+\vert\beta\vert^2}\langle g^*_{l,0}\eta_l\hat{\mathcal{O}}\rangle_0$
$\langle\beta\vert\, c_0^\dagger c_{L+1}^\dagger\hat{\mathcal{O}}\,\vert\beta\rangle$	$\frac{1}{4}\frac{1-\vert\beta\vert^2}{1+\vert\beta\vert^2}\langle\hat{\mathcal{O}}\rangle_0 - g^*_{l,0}g_{k,L+1}\langle\eta_l\eta_k^\dagger\hat{\mathcal{O}}\rangle_0$	$\frac{\mathrm{Re}[\beta]}{1+\vert\beta\vert^2}\langle g^*_{l,L+1}\eta_l\hat{\mathcal{O}}\rangle_0 - \frac{i\mathrm{Im}[\beta]}{1+\vert\beta\vert^2}\langle g^*_{l,0}\eta_l\hat{\mathcal{O}}\rangle_0$
	$\hat{\mathcal{O}}$ has no $\bar{\gamma}_0$ and γ_{L+1}	
$\langle\beta\vert\,\gamma_0\hat{\mathcal{O}}\,\vert\beta\rangle$	$\frac{2\mathrm{Re}[\beta]}{1+\vert\beta\vert^2}\,\langle 0\vert\,\hat{\mathcal{O}}\,\vert 0\rangle$	0
$\langle\beta\vert\,\bar{\gamma}_0\hat{\mathcal{O}}\,\vert\beta\rangle$	0	$-2ig^*_{k,0}\,\langle 0\vert\,\eta_k\hat{\mathcal{O}}\,\vert 0\rangle$

7.4 Reduced Density matrix

In this section, we calculate the density matrix and reduced density matrix (RDM) of the particular states introduced previously. We are going to use the configurational basis result of 7.2.4 and coherent basis formulation to calculate the density matrix and RDM. The RDM will be presented in both coherent basis and operator form. The operator form of RDM is useful to calculate the entanglement content of the states, while the coherent basis form of the RDM can be used to study the formation probabilities. In subsection 7.4.1, we start with the β-broken parity state (7.31). We calculate the total density matrix and then the RDM in coherent basis and operator format. In subsections 7.4.2, 7.4.3 and 7.4.4 we present the same calculations for the states $|0\rangle_\eta$, $|\emptyset\rangle$ and $|G_\pm\rangle$, respectively.

7.4.1 β parity broken state

We start by calculating the reduced density matrix for the state $|\beta\rangle$ defined in (7.31). The total density matrix of a particular state $|\psi\rangle$ is defined as $\rho = |\psi\rangle\langle\psi|$. We prefer to calculate the density matrix for the state $|\beta\rangle$ explicitly in an exponential form using the

definition (2.53). With the +1 parity for the state $|0\rangle_\eta$, the density matrix has the form

$$\rho^\beta = |\beta\rangle\langle\beta| = |C^\beta|^2 e^{\frac{1}{2}R_{ij}c_i^\dagger c_j^\dagger}(1+\beta\mathfrak{M}_{0k}c_k^\dagger)\,|0\rangle_c\,{}_c\langle 0|\,(1+\beta^*\mathfrak{M}^*_{0l}c_l)e^{-\frac{1}{2}R^*_{ij}c_ic_j}, \tag{7.67}$$

where $|C^\beta|^2 = \left((1+|\beta|^2)\sqrt{\det[\mathbf{I}+\mathbf{R}^\dagger\mathbf{R}]}\right)^{-1}$ and $\mathfrak{M} = \mathbf{h}^*.\mathbf{R} + \mathbf{g}^*$. To proceed, we use the Fermionic coherent state defined as

$$|\boldsymbol{\xi}\rangle = |\xi_1\xi_2\cdots\xi_N\rangle = e^{-\sum_{k=1}^N \xi_k c_k^\dagger}\,|0\rangle_c\,, \tag{7.68}$$

where ξ_k are Grassmann variables. Therefore, we can write (following similar procedure as [13])

$$\langle\boldsymbol{\xi}|\,\rho^\beta\,|\boldsymbol{\xi}'\rangle = \rho^\beta(\boldsymbol{\xi},\boldsymbol{\xi}') = |C^\beta|^2 e^{\frac{1}{2}R_{ij}\bar{\xi}_i\bar{\xi}_j}(1+\beta\mathfrak{M}_{0k}\bar{\xi}_k)(\beta^*\mathfrak{M}^*_{0l}\xi'_l+1)e^{-\frac{1}{2}R^*_{nm}\xi'_n\xi'_m}. \tag{7.69}$$

To obtain the reduced density matrix (RDM), we divide the system into two parts (subsystem) **1** and **2**. Here, we denote parts of any matrix that correspond to the subsystem **1** (**2**) with the subscript 1 (2)[3] . We trace out the subsystem **2** to find the RDM for subsystem **1**, $\rho_{\mathbf{1}} = \mathrm{tr}_{\mathbf{2}}\rho$. In order to do so, we use the trace formula for operators in the coherent basis. Therefore, we have:

$$\rho^\beta_{\mathbf{1}}(\boldsymbol{\xi},\boldsymbol{\xi}') = \int\prod_{l\in\mathbf{2}}\mathrm{d}\bar{\xi}_l\mathrm{d}\xi_l\; e^{-\sum\limits_{n\in\mathbf{2}}\bar{\xi}_n\xi_n}\,\langle\xi_1,\cdots,\xi_k,-\xi_{k+1},\cdots,-\xi_L|\,\rho^\beta\,|\xi'_1,\cdots,\xi'_k,\xi_{k+1},\cdots,\xi_L\rangle\,, \tag{7.70}$$

where $\xi_1,\cdots,\xi_k$ belong to the subsystem **1** and $\xi_{k+1},\cdots,\xi_L$ belong to the subsystem 2. For the details of calculation, see appendix D. The final result after partial tracing the (7.69) is:

$$\rho^\beta_{\mathbf{1}}(\boldsymbol{\xi},\boldsymbol{\xi}') = \mathcal{C}^\beta\Big[\Big(\frac{1}{\beta}+\boldsymbol{\mathcal{L}}_1.\bar{\boldsymbol{\xi}}+\boldsymbol{\mathcal{L}}_2.\boldsymbol{\xi}'\Big)\Big(\frac{1}{\beta^*}+\boldsymbol{\mathcal{L}}_3.\bar{\boldsymbol{\xi}}+\boldsymbol{\mathcal{L}}_4.\boldsymbol{\xi}'\Big)-\mathrm{Pf}[\boldsymbol{\mathcal{W}}]\Big]e^{\frac{1}{2}\begin{pmatrix}\bar{\xi} & \xi'\end{pmatrix}\boldsymbol{\Omega}\begin{pmatrix}\bar{\xi}\\ \xi'\end{pmatrix}}, \tag{7.71}$$

where the $\mathcal{C}^\beta$ and the introduced matrices are given by:

$$\mathcal{C}^\beta = \frac{|\beta|^2\sqrt{\det\left[\mathbf{I}+{\mathbf{R}_{22}}^\dagger\mathbf{R}_{22}\right]}}{(1+|\beta|^2)\sqrt{\det\left[\mathbf{I}+\mathbf{R}^\dagger\mathbf{R}\right]}}, \tag{7.72a}$$

$$\boldsymbol{\Omega} = \begin{pmatrix}\mathbf{R}_{11} & 0\\ 0 & -{\mathbf{R}_{11}}^*\end{pmatrix} + \begin{pmatrix}\mathbf{R}_{12} & 0\\ 0 & {\mathbf{R}_{12}}^*\end{pmatrix}\boldsymbol{\mathcal{A}}^{-1}\begin{pmatrix}{\mathbf{R}_{12}}^T & 0\\ 0 & {\mathbf{R}_{12}}^\dagger\end{pmatrix}, \tag{7.72b}$$

[3] For instance, the $\mathbf{A}_{12}$ stands for the sub-matrix of $\mathbf{A}$ that rows and columns belong to subsystem 1 and 2 respectively

$$\begin{pmatrix} \boldsymbol{\mathcal{L}}_1 & \boldsymbol{\mathcal{L}}_2 \\ \boldsymbol{\mathcal{L}}_3 & \boldsymbol{\mathcal{L}}_4 \end{pmatrix} = \begin{pmatrix} \boldsymbol{\mathfrak{M}}_1 & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\mathfrak{M}}_1^* \end{pmatrix} + \begin{pmatrix} \boldsymbol{\mathfrak{M}}_2 & \mathbf{0} \\ \mathbf{0} & -\boldsymbol{\mathfrak{M}}_2^* \end{pmatrix} \boldsymbol{\mathcal{A}}^{-1} \begin{pmatrix} \mathbf{R}_{12}^T & \mathbf{0} \\ \mathbf{0} & \mathbf{R}_{12}^\dagger \end{pmatrix}, \tag{7.72c}$$

$$\boldsymbol{\mathcal{W}} = \begin{pmatrix} \boldsymbol{\mathfrak{M}}_2 & \mathbf{0} \\ \mathbf{0} & -\boldsymbol{\mathfrak{M}}_2^* \end{pmatrix} \boldsymbol{\mathcal{A}}^{-T} \begin{pmatrix} \boldsymbol{\mathfrak{M}}_2^T & \mathbf{0} \\ \mathbf{0} & -\boldsymbol{\mathfrak{M}}_2^\dagger \end{pmatrix}, \tag{7.72d}$$

$$\boldsymbol{\mathcal{A}} = \begin{pmatrix} \mathbf{R}_{22} & -\mathbf{I} \\ \mathbf{I} & -\mathbf{R}_{22}^* \end{pmatrix}. \tag{7.72e}$$

It is useful also to have the RDM in the operator format (for example to calculate the Rényi entanglement entropy). To derive the operator form for $\rho_{\mathbf{1}}$ from equation (7.71), we rewrite the exponential term as

$$\mathrm{Exp}\Big[\tfrac{1}{2}\begin{pmatrix} \bar{\xi} & \xi' \end{pmatrix} \boldsymbol{\Omega} \begin{pmatrix} \bar{\xi} \\ \xi' \end{pmatrix}\Big] = \mathrm{Exp}\Big[\tfrac{1}{2}\mathcal{X}_{ij}\bar{\xi}_i\bar{\xi}_j\Big]\mathrm{Exp}\Big[\mathcal{Y}_{ij}\bar{\xi}_i\xi'_j\Big]\ \mathrm{Exp}\Big[\tfrac{1}{2}\mathcal{Z}_{ij}\xi'_i\xi'_j\Big] \tag{7.73}$$

with properly defined matrices $\mathcal{X}$, $\mathcal{Y}$ and $\mathcal{Z}$. Using the relations $c_ic_j\,|\boldsymbol{\xi}\rangle = \xi_i\xi_j\,|\boldsymbol{\xi}\rangle$ and $\langle\boldsymbol{\xi}|\,c_i^\dagger c_j^\dagger = \langle\boldsymbol{\xi}|\,\bar{\xi}_i\bar{\xi}_j$, one can replace $\bar{\xi}_i\bar{\xi}_j$ with $c_i^\dagger c_j^\dagger$ and $\xi'_i\xi'_j$ with c_ic_j in the left and right exponentials. The cross term can be rewritten $\mathcal{Y}_{ij}\bar{\xi}_i\xi'_j \;\to\; \ln(\boldsymbol{\mathcal{Y}})_{ij}c_i^\dagger c_j$. The final operator form of RDM (7.71) is given as:

$$\begin{aligned}\rho_{\mathbf{1}}^\beta(c,c^\dagger) = \mathcal{C}^\beta\, e^{\frac{1}{2}\begin{pmatrix}\mathbf{c}^\dagger & \mathbf{c}\end{pmatrix}\boldsymbol{\mathcal{M}}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^\dagger\end{pmatrix}}\, e^{\frac{1}{2}\mathrm{tr}\ln(\frac{1}{2}\boldsymbol{\Omega}_{12}-\frac{1}{2}\boldsymbol{\Omega}_{21}^T)}\Big[\mathrm{Pf}[\boldsymbol{\mathcal{W}}] - \boldsymbol{\mathcal{L}}_3\boldsymbol{\mathcal{T}}_{22}\boldsymbol{\mathcal{L}}_2 \\ + \Big(\boldsymbol{\mathcal{L}}_1\boldsymbol{\mathcal{T}}_{22}\mathbf{c}^\dagger + (\boldsymbol{\mathcal{L}}_1\boldsymbol{\mathcal{T}}_{21}+\boldsymbol{\mathcal{L}}_2)\mathbf{c} + \frac{1}{\beta}\Big)\Big(\boldsymbol{\mathcal{L}}_3\boldsymbol{\mathcal{T}}_{22}\mathbf{c}^\dagger + (\boldsymbol{\mathcal{L}}_4+\boldsymbol{\mathcal{L}}_3\boldsymbol{\mathcal{T}}_{21})\mathbf{c} + \frac{1}{\beta^*}\Big)\Big]\end{aligned} \tag{7.74}$$

where

$$\boldsymbol{\mathcal{M}} = \ln\boldsymbol{\mathcal{T}}; \quad \boldsymbol{\mathcal{T}} = \begin{pmatrix} \frac{1}{2}\boldsymbol{\Omega}_{12} - \frac{1}{2}\boldsymbol{\Omega}_{21}{}^T + 2\boldsymbol{\Omega}_{11}(\boldsymbol{\Omega}_{12}^T - \boldsymbol{\Omega}_{21})^{-T}\boldsymbol{\Omega}_{22} & 2\boldsymbol{\Omega}_{11}(\boldsymbol{\Omega}_{12}^T - \boldsymbol{\Omega}_{21})^{-T} \\ 2(\boldsymbol{\Omega}_{12}^T - \boldsymbol{\Omega}_{21})^{-T}\boldsymbol{\Omega}_{22} & 2(\boldsymbol{\Omega}_{12}^T - \boldsymbol{\Omega}_{21})^{-T} \end{pmatrix}, \tag{7.75a}$$

$$\boldsymbol{\Omega} = \begin{pmatrix} \mathbf{R}_{11} & 0 \\ 0 & -\mathbf{R}_{11}{}^{*} \end{pmatrix} + \begin{pmatrix} \mathbf{R}_{12} & 0 \\ 0 & \mathbf{R}_{12}{}^{*} \end{pmatrix} \boldsymbol{\mathcal{A}}^{-1} \begin{pmatrix} \mathbf{R}_{12}{}^{T} & 0 \\ 0 & \mathbf{R}_{12}{}^{\dagger} \end{pmatrix}; \qquad \boldsymbol{\mathcal{A}} = \begin{pmatrix} \mathbf{R}_{22} & -\mathbf{I} \\ \mathbf{I} & -\mathbf{R}_{22}^{*} \end{pmatrix} \tag{7.75b}$$

$$\boldsymbol{\mathcal{W}} = \begin{pmatrix} \boldsymbol{\mathfrak{M}}_2 & \mathbf{0} \\ \mathbf{0} & -\boldsymbol{\mathfrak{M}}_2^{*} \end{pmatrix} \boldsymbol{\mathcal{A}}^{-T} \begin{pmatrix} \boldsymbol{\mathfrak{M}}_2^{T} & \mathbf{0} \\ \mathbf{0} & -\boldsymbol{\mathfrak{M}}_2^{\dagger} \end{pmatrix} \tag{7.75c}$$

$$\begin{pmatrix} \boldsymbol{\mathcal{L}}_1 & \boldsymbol{\mathcal{L}}_2 \\ \boldsymbol{\mathcal{L}}_3 & \boldsymbol{\mathcal{L}}_4 \end{pmatrix} = \begin{pmatrix} \boldsymbol{\mathfrak{M}}_1 & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\mathfrak{M}}_1^{*} \end{pmatrix} + \begin{pmatrix} \boldsymbol{\mathfrak{M}}_2 & \mathbf{0} \\ \mathbf{0} & -\boldsymbol{\mathfrak{M}}_2^{*} \end{pmatrix} \boldsymbol{\mathcal{A}}^{-1} \begin{pmatrix} \mathbf{R}_{12}^{T} & \mathbf{0} \\ \mathbf{0} & \mathbf{R}_{12}^{\dagger} \end{pmatrix}. \tag{7.75d}$$

Also, $\boldsymbol{\mathcal{T}}_{11}$, $\boldsymbol{\mathcal{T}}_{12}$, $\boldsymbol{\mathcal{T}}_{21}$ and $\boldsymbol{\mathcal{T}}_{22}$ stand for the sub-matrices (blocks) of matrix $\boldsymbol{\mathcal{T}}$. In the above expression, to move the exponential with fermionic operators, we have used the following relation, coming from Baker-Hausdorff formula,

$$F^{-1} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^{\dagger} \end{pmatrix} F = \boldsymbol{\mathcal{T}} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^{\dagger} \end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^{\dagger} \end{pmatrix} F = F \boldsymbol{\mathcal{T}} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^{\dagger} \end{pmatrix}; \qquad F = e^{\frac{1}{2}\begin{pmatrix} \mathbf{c}^{\dagger} & \mathbf{c} \end{pmatrix} \boldsymbol{\mathcal{M}} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^{\dagger} \end{pmatrix}}. \tag{7.76}$$

In the expression of RDM, having all the creation and annihilation operators in the argument of exponential is preferred (some of calculations would be simplified). For this reason, we present another calculation of ρ_1^{β} in the appendix D, where using a trick, we managed to get the RDM with two exponentials. The above equations are valid for the RDM of $|\beta\rangle$-state, which also means, for any given bi partition, one can use (7.74). However, it should be noted that the spin and fermion representations for solvable quantum chains lead to different RDMs. For more details see section 7.4.5.

We can propose an ansatz to write the RDM for $|\beta\rangle$ in term of correlation matrix. Although computationally favorable, the down side of such an ansatz is that we could only use it for a particular type of bipartition. while we can not apply Wick theorem to $|\beta\rangle$, one can use the $\boldsymbol{\Gamma}^{\beta}$ matrix to calculate the RDM of a subsystem which starts from one boundary. One has to make an adjustment to the Peschel method. Such a procedure for $\beta = \pm 1$ has been shown in [156]; here we are extending that result.

Since the $\boldsymbol{\Gamma}^{\beta}$ matrix is a skew symmetric matrix it can be written in a block form

using an orthogonal matrix $\mathbf{V}$ as:

$$\mathbf{V}\boldsymbol{\Gamma}^{\beta}\mathbf{V}^{T} = \begin{pmatrix} \mathbf{0} & i\boldsymbol{\nu} \\ -i\boldsymbol{\nu} & \mathbf{0} \end{pmatrix}, \tag{7.77}$$

where $\boldsymbol{\nu}$ is a diagonal matrix. Then, we can define the following fermionic operators:

$$\begin{pmatrix} \boldsymbol{d}^{\dagger} \\ \boldsymbol{d} \end{pmatrix} = \frac{1}{\sqrt{2}}\mathbf{W}\begin{pmatrix} \boldsymbol{\gamma} \\ \bar{\boldsymbol{\gamma}} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} \mathbf{I} & i\mathbf{I} \\ \mathbf{I} & -i\mathbf{I} \end{pmatrix}\mathbf{V}\begin{pmatrix} \boldsymbol{\gamma} \\ \bar{\boldsymbol{\gamma}} \end{pmatrix}. \tag{7.78}$$

Similar to the results in [156], one can make an ansatz for the RDM of the subsystem $\mathbf{1}$. To be precise, we are assuming that the subsystem $\mathbf{1}$ is a connected bipartite of the system starting from site 0 to ℓ. The ansatz should have a form like below with respect to the operators that diagonalize the $\boldsymbol{\Gamma}^{\beta}$ matrix.

$$\rho_{\mathbf{1}}^{\beta}(d, d^{\dagger}) = \mathrm{g}(d_0, d_0^{\dagger}, d_0^{\dagger}d_0) \times \prod_{k=1}^{\ell}\Big(\frac{1+\nu_k}{2}d_k^{\dagger}d_k + \frac{1-\nu_k}{2}d_k d_k^{\dagger}\Big),$$

where g is an arbitrary function to be determined. From correlation matrices (section 7.3), we can realize that

$$\mathrm{g}(c_0, c_0^{\dagger}, c_0^{\dagger}c_0) = \frac{\mathrm{Re}[\beta]}{1+|\beta|^2}(c_0^{\dagger} + c_0) + \frac{1}{2}\mathbf{I}. \tag{7.79}$$

This ansatz satisfies the expectations of the state $|\beta\rangle$ including one point functions (7.62). It is easy to show that $\boldsymbol{c}^{\dagger} + \boldsymbol{c} = \sqrt{2}\Big(\boldsymbol{W}_{11}^{\dagger}\boldsymbol{d}^{\dagger} + \boldsymbol{W}_{11}^{T}\boldsymbol{d}\Big)$, where $\boldsymbol{W}$ is the unitary transformation which diagonalizes the matrix $\boldsymbol{\Gamma}^{\beta}$. Then, in terms of d and $d^{\dagger}$ operators we have:

$$\rho_{\mathbf{1}}^{\beta}(d, d^{\dagger}) = \frac{\mathrm{Re}[\beta]}{1+|\beta|^2}\Big(\tfrac{\sqrt{2}}{2}d_0 + \tfrac{\sqrt{2}}{2}d_0^{\dagger} + \tfrac{1}{2}\mathbf{I}\Big) \times \prod_{k=1}^{\ell}\Big(\frac{1+\nu_k}{2}d_k^{\dagger}d_k + \frac{1-\nu_k}{2}d_k d_k^{\dagger}\Big), \tag{7.80}$$

The ansatz (7.80) respects the generalized Wick's theorem, which means that this RDM produces all the correlation functions correctly. As an example, one point function is not necessarily zero for the $|\beta\rangle$:

$$\langle d_k^{\dagger}\rangle_{\beta} = \frac{1}{\sqrt{2}}\frac{\mathrm{Re}[\beta]}{1+|\beta|^2}\delta_{k,0}, \tag{7.81}$$

$$\langle d_k\rangle_{\beta} = \frac{1}{\sqrt{2}}\frac{\mathrm{Re}[\beta]}{1+|\beta|^2}\delta_{k,0}. \tag{7.82}$$

Based on (7.65), (7.66) and (3.2), the first row and column of matrix $\boldsymbol{\Gamma}^{\beta}$ is zero which evidently means it has a zero eigenvalue, $\nu_0 = 0$. From the earlier statement it can be

inferred that the matrix which diagonalizes the $\mathbf{\Gamma}^{\beta}$ -called $\boldsymbol{W}$- has the following form:

$$\boldsymbol{W}=\begin{pmatrix}\boldsymbol{W}_{11} & \boldsymbol{W}_{12}\\ \boldsymbol{W}_{11}{}^{*} & \boldsymbol{W}_{12}{}^{*}\end{pmatrix};\qquad \boldsymbol{W}_{11}=\begin{pmatrix}1 & 0 & \cdots & 0\\ 0 & & \boldsymbol{\omega} & \\ \vdots & & & \\ 0 & & & \end{pmatrix}. \tag{7.83}$$

The reason we have defined the $\boldsymbol{W}$ as above is that the $\boldsymbol{d}^{\dagger}$ and $\boldsymbol{d}$ should be related with a conjugate transpose transformation. From (7.77), The $\boldsymbol{W}$ and $\boldsymbol{V}$ matrices are related by $\boldsymbol{W}\propto\begin{pmatrix}\mathbf{I} & i\mathbf{I}\\ \mathbf{I} & -i\mathbf{I}\end{pmatrix}\mathbf{V}$, which means we can write:

$$\begin{pmatrix}\boldsymbol{d}^{\dagger}\\ \boldsymbol{d}\end{pmatrix}=\frac{1}{\sqrt{2}}\begin{pmatrix}\boldsymbol{W}_{11}\boldsymbol{\gamma}+\boldsymbol{W}_{12}\bar{\boldsymbol{\gamma}}\\ \boldsymbol{W}^{*}_{11}\boldsymbol{\gamma}+\boldsymbol{W}^{*}_{12}\bar{\boldsymbol{\gamma}}\end{pmatrix}. \tag{7.84}$$

We know that $\langle\bar{\gamma}_i\rangle_\beta=0$ and $\langle\gamma_i\rangle_\beta=\delta_{i,0}$, then we can write $\langle d_k^{\dagger}\rangle_\beta=(\boldsymbol{W}_{11})_{k,0}$. Making use of the relation (7.83), we have $\langle d_k^{\dagger}\rangle_\beta\propto\delta_{k,0}$. For the $\langle d_k\rangle_\beta$ case, we use the fact that $\boldsymbol{d}$ and $\boldsymbol{d}^{\dagger}$ are related by a conjugation, which means that $\langle d_k\rangle_\beta\propto\delta_{k,0}$ and the proof is complete.

Note that, the above calculation is also valid for states $|G_+\rangle$, $|G_-\rangle$ and any state created from the action of $\eta^{\dagger}$'s on these states. Consequently, with a proper $\mathbf{\Gamma}$ matrix, a similar ansatz to (7.80) can be used to study the entanglement for all the states belonging to the four sectors created with $|G_\pm\rangle$ as introduced in subsection 7.2.6.

7.4.2 Vacuum state

As it was mentioned before the limit $\beta\to 0$ in the $|\beta\rangle$, gives the $|0\rangle_\eta$. Equivalently, $\lim_{\beta\to 0}\rho^{\beta}=\rho^{0}=|0\rangle_{\eta\,\eta}\langle 0|$. Simply, we are going to apply this limit on the results of subsection 7.4.1 to find the required quantities in this subsection. For instance, in the limit $\beta\to 0$, the only nonzero term in (7.71) is $|\mathcal{C}^{\beta}|^2\frac{1}{|\beta|^2}$. Therefore for the RDM of vacuum state in the coherent basis we have:

$$\rho_{\mathbf{1}}^{0}(\boldsymbol{\xi},\boldsymbol{\xi}')=\frac{\sqrt{\det\left[\mathbf{I}+{\mathbf{R}_{22}}^{\dagger}\mathbf{R}_{22}\right]}}{\sqrt{\det\left[\mathbf{I}+\mathbf{R}^{\dagger}\mathbf{R}\right]}}e^{\frac{1}{2}\begin{pmatrix}\bar{\xi} & \xi'\end{pmatrix}\mathbf{\Omega}\begin{pmatrix}\bar{\xi}\\ \xi'\end{pmatrix}}, \tag{7.85}$$

where:

$$\boldsymbol{\mathcal{A}} = \begin{pmatrix} \mathbf{R}_{22} & -\mathbf{I} \\ \mathbf{I} & -\mathbf{R}_{22}^{*} \end{pmatrix}, \tag{7.86a}$$

$$\boldsymbol{\Omega} = \begin{pmatrix} \mathbf{R}_{11} & 0 \\ 0 & -\mathbf{R}_{11}{}^{*} \end{pmatrix} + \begin{pmatrix} \mathbf{R}_{12} & 0 \\ 0 & \mathbf{R}_{12}{}^{*} \end{pmatrix} \boldsymbol{\mathcal{A}}^{-1} \begin{pmatrix} \mathbf{R}_{12}{}^{T} & 0 \\ 0 & \mathbf{R}_{12}{}^{\dagger} \end{pmatrix}. \tag{7.86b}$$

The operator form of RDM reads as

$$\rho_{\mathbf{1}}^{0}(c, c^{\dagger}) = \frac{\sqrt{\det\left[\mathbf{I} + \mathbf{R}_{22}{}^{\dagger}\mathbf{R}_{22}\right]}}{\sqrt{\det\left[\mathbf{I} + \mathbf{R}^{\dagger}\mathbf{R}\right]}} e^{\frac{1}{2}\begin{pmatrix} \mathbf{c}^{\dagger} & \mathbf{c} \end{pmatrix} \boldsymbol{\mathcal{M}} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^{\dagger} \end{pmatrix}} e^{\frac{1}{2}\mathrm{tr}\ln(\frac{1}{2}\boldsymbol{\Omega}_{12} - \frac{1}{2}\boldsymbol{\Omega}_{21}^{T})}, \tag{7.87}$$

where

$$\boldsymbol{\mathcal{M}} = \ln \boldsymbol{\mathcal{T}}; \quad \boldsymbol{\mathcal{T}} = \begin{pmatrix} \frac{1}{2}\boldsymbol{\Omega}_{12} - \frac{1}{2}\boldsymbol{\Omega}_{21}{}^{T} + 2\boldsymbol{\Omega}_{11}(\boldsymbol{\Omega}_{12}^{T} - \boldsymbol{\Omega}_{21})^{-T}\boldsymbol{\Omega}_{22} & 2\boldsymbol{\Omega}_{11}(\boldsymbol{\Omega}_{12}^{T} - \boldsymbol{\Omega}_{21})^{-T} \\ 2(\boldsymbol{\Omega}_{12}^{T} - \boldsymbol{\Omega}_{21})^{-T}\boldsymbol{\Omega}_{22} & 2(\boldsymbol{\Omega}_{12}^{T} - \boldsymbol{\Omega}_{21})^{-T} \end{pmatrix}, \tag{7.88a}$$

$$\boldsymbol{\Omega} = \begin{pmatrix} \mathbf{R}_{11} & 0 \\ 0 & -\mathbf{R}_{11}^{*} \end{pmatrix} + \begin{pmatrix} \mathbf{R}_{12} & 0 \\ 0 & \mathbf{R}_{12}^{*} \end{pmatrix} \boldsymbol{\mathcal{A}}^{-1} \begin{pmatrix} \mathbf{R}_{12}^{T} & 0 \\ 0 & \mathbf{R}_{12}^{\dagger} \end{pmatrix}; \qquad \boldsymbol{\mathcal{A}} = \begin{pmatrix} \mathbf{R}_{22} & -\mathbf{I} \\ \mathbf{I} & -\mathbf{R}_{22}^{*} \end{pmatrix}. \tag{7.88b}$$

Since one can use Wick theorem for the state $|0\rangle_{\eta}$, the RDM can be written in terms of Majorana fermions and their correlations (introduced in section 7.3) in subsystem **1**. The reduced density matrix can be written as [14]:

$$\rho_{\mathbf{1}}^{0}(\boldsymbol{\gamma}, \bar{\boldsymbol{\gamma}}) = [\det\frac{\mathbf{I} - \boldsymbol{\Gamma}_{\mathbf{1}}^{\mathbf{0}}}{2}]^{\frac{1}{2}} e^{\frac{1}{4}\begin{pmatrix} \boldsymbol{\gamma} & \bar{\boldsymbol{\gamma}} \end{pmatrix} \ln\frac{\mathbf{I} + \boldsymbol{\Gamma}_{\mathbf{1}}^{\mathbf{0}}}{\mathbf{I} - \boldsymbol{\Gamma}_{\mathbf{1}}^{\mathbf{0}}} \begin{pmatrix} \boldsymbol{\gamma} \\ \bar{\boldsymbol{\gamma}} \end{pmatrix}}, \tag{7.89}$$

where the $\begin{pmatrix} \boldsymbol{\gamma} & \bar{\boldsymbol{\gamma}} \end{pmatrix}$ contains all the Majorana fermions of subsystem **1**. The $\boldsymbol{\Gamma}_{\mathbf{1}}^{\mathbf{0}}$ stands for the correlation matrix defined in section 7.3 calculated for the vacuum state and subsystem **1**. The constant in (7.89) can be simplified as:

$$\det[\frac{\mathbf{I} - \boldsymbol{\Gamma}_{\mathbf{1}}^{\mathbf{0}}}{2}] = \det[\mathbf{K}_{\mathbf{1}}^{\mathbf{0}}]\det[\frac{\bar{\mathbf{K}}_{1}^{0} - \mathbf{G}_{\mathbf{1}}^{\mathbf{0}}.\mathbf{K}_{\mathbf{1}}^{\mathbf{0}-1}.\mathbf{G}_{\mathbf{1}}^{\mathbf{0}T}}{4}]. \tag{7.90}$$

7.4.3 ZME state

The ZME state can be obtained by the limit $|\emptyset\rangle = \lim_{\beta\to\infty} |\beta\rangle$. Therefore, the RDM $\rho^{\emptyset} = |\emptyset\rangle\langle\emptyset|$ in the operator form will be the large β limit of the results of the subsection 7.4.1.

$$\begin{aligned}\rho_{\mathbf{1}}^{\beta}(c,c^\dagger) = \mathcal{C}^{\emptyset}\, e^{\frac{1}{2}\begin{pmatrix}\mathbf{c}^\dagger & \mathbf{c}\end{pmatrix}\boldsymbol{\mathcal{M}}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^\dagger\end{pmatrix}} e^{\frac{1}{2}\mathrm{tr}\ln(\frac{1}{2}\boldsymbol{\Omega}_{12}-\frac{1}{2}\boldsymbol{\Omega}_{21}^T)}\Big[\mathrm{Pf}[\boldsymbol{\mathcal{W}}] - \boldsymbol{\mathcal{L}}_3\boldsymbol{\mathcal{T}}_{22}\boldsymbol{\mathcal{L}}_2 \\ + \Big(\boldsymbol{\mathcal{L}}_1\boldsymbol{\mathcal{T}}_{22}\boldsymbol{c}^\dagger + (\boldsymbol{\mathcal{L}}_1\boldsymbol{\mathcal{T}}_{21}+\boldsymbol{\mathcal{L}}_2)\boldsymbol{c}\Big)\Big(\boldsymbol{\mathcal{L}}_3\boldsymbol{\mathcal{T}}_{22}\boldsymbol{c}^\dagger + (\boldsymbol{\mathcal{L}}_4+\boldsymbol{\mathcal{L}}_3\boldsymbol{\mathcal{T}}_{21})\boldsymbol{c}\Big)\Big]\end{aligned} \tag{7.91}$$

where

$$\boldsymbol{\mathcal{W}} = \begin{pmatrix}\mathfrak{M}_2 & \mathbf{0}\\ \mathbf{0} & -\mathfrak{M}_2^*\end{pmatrix}\boldsymbol{\mathcal{A}}^{-T}\begin{pmatrix}\mathfrak{M}_2^T & \mathbf{0}\\ \mathbf{0} & -\mathfrak{M}_2^\dagger\end{pmatrix}; \qquad \boldsymbol{\mathcal{A}} = \begin{pmatrix}\mathbf{R}_{22} & -\mathbf{I}\\ \mathbf{I} & -\mathbf{R}_{22}^*\end{pmatrix}, \tag{7.92a}$$

$$\boldsymbol{\mathcal{M}} = \ln\boldsymbol{\mathcal{T}}; \quad \boldsymbol{\mathcal{T}} = \begin{pmatrix}\frac{1}{2}\boldsymbol{\Omega}_{12} - \frac{1}{2}\boldsymbol{\Omega}_{21}{}^T + 2\boldsymbol{\Omega}_{11}(\boldsymbol{\Omega}_{12}^T-\boldsymbol{\Omega}_{21})^{-T}\boldsymbol{\Omega}_{22} & 2\boldsymbol{\Omega}_{11}(\boldsymbol{\Omega}_{12}^T-\boldsymbol{\Omega}_{21})^{-T}\\ 2(\boldsymbol{\Omega}_{12}^T-\boldsymbol{\Omega}_{21})^{-T}\boldsymbol{\Omega}_{22} & 2(\boldsymbol{\Omega}_{12}^T-\boldsymbol{\Omega}_{21})^{-T}\end{pmatrix}, \tag{7.92b}$$

$$\boldsymbol{\Omega} = \begin{pmatrix}\mathbf{R}_{11} & 0\\ 0 & -\mathbf{R}_{11}{}^*\end{pmatrix} + \begin{pmatrix}\mathbf{R}_{12} & 0\\ 0 & \mathbf{R}_{12}{}^*\end{pmatrix}\boldsymbol{\mathcal{A}}^{-1}\begin{pmatrix}\mathbf{R}_{12}{}^T & 0\\ 0 & \mathbf{R}_{12}{}^\dagger\end{pmatrix}, \tag{7.92c}$$

$$\begin{pmatrix}\boldsymbol{\mathcal{L}}_1 & \boldsymbol{\mathcal{L}}_2\\ \boldsymbol{\mathcal{L}}_3 & \boldsymbol{\mathcal{L}}_4\end{pmatrix} = \begin{pmatrix}\mathfrak{M}_1 & \mathbf{0}\\ \mathbf{0} & \mathfrak{M}_1^*\end{pmatrix} + \begin{pmatrix}\mathfrak{M}_2 & \mathbf{0}\\ \mathbf{0} & -\mathfrak{M}_2^*\end{pmatrix}\boldsymbol{\mathcal{A}}^{-1}\begin{pmatrix}\mathbf{R}_{12}^T & \mathbf{0}\\ \mathbf{0} & \mathbf{R}_{12}^\dagger\end{pmatrix}. \tag{7.92d}$$

The above equation is lengthy and calculation of entanglement seem difficult with the above RDM. However, since the ZME state has an opposite parity with respect to $|0\rangle_\eta$. One can use the *Tilda transformation* introduced in the subsection 7.2.4 to write the ZME state as:

$$|\emptyset\rangle = C^{\emptyset} e^{\frac{1}{2}\sum_{i,j} R^{\emptyset}_{ij}\tilde{c}_i^\dagger\tilde{c}_j^\dagger}|\tilde{0}\rangle_c \tag{7.93}$$

with properly defined $\mathbf{R}^{\emptyset}$ matrix and constant $C^{\emptyset}$. The above Gaussian form for the ZME state will simplify some of the calculations exceedingly. For instance, using the (7.93), it is possible to write a shorter notation for RDM as:

$$\rho_{\mathbf{1}}^{\emptyset}(c,c^\dagger) = C^{\emptyset\prime} e^{\frac{1}{2}\begin{pmatrix}\mathbf{c}^\dagger & \mathbf{c}\end{pmatrix}\mathcal{M}^{\emptyset}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^\dagger\end{pmatrix}}, \tag{7.94}$$

where $C^{\emptyset'}$ is the normalization factor and $\boldsymbol{\mathcal{M}}^{\emptyset} = \ln \boldsymbol{\mathcal{T}}^{\emptyset}$ which we have:

$$\boldsymbol{\mathcal{T}}^{\emptyset} = \begin{pmatrix} \frac{1}{2}\boldsymbol{\Omega}^{\emptyset}_{12} - \frac{1}{2}{\boldsymbol{\Omega}^{\emptyset}_{21}}^{T} + 2\boldsymbol{\Omega}^{\emptyset}_{11}({\boldsymbol{\Omega}^{\emptyset}_{12}}^{T} - \boldsymbol{\Omega}^{\emptyset}_{21})^{-T}\boldsymbol{\Omega}^{\emptyset}_{22} & 2\boldsymbol{\Omega}^{\emptyset}_{11}({\boldsymbol{\Omega}^{\emptyset}_{12}}^{T} - \boldsymbol{\Omega}^{\emptyset}_{21})^{-T} \\ 2({\boldsymbol{\Omega}^{\emptyset}_{12}}^{T} - \boldsymbol{\Omega}^{\emptyset}_{21})^{-T}\boldsymbol{\Omega}^{\emptyset}_{22} & 2({\boldsymbol{\Omega}^{\emptyset}_{12}}^{T} - \boldsymbol{\Omega}^{\emptyset}_{21})^{-T} \end{pmatrix}, \tag{7.95a}$$

$$\boldsymbol{\Omega}^{\emptyset} = \begin{pmatrix} \mathbf{R}^{\emptyset}_{11} & 0 \\ 0 & -{\mathbf{R}^{\emptyset}_{11}}^{*} \end{pmatrix} + \begin{pmatrix} \mathbf{R}^{\emptyset}_{12} & 0 \\ 0 & {\mathbf{R}^{\emptyset}_{12}}^{*} \end{pmatrix} {\boldsymbol{\mathcal{A}}^{\emptyset}}^{-1} \begin{pmatrix} {\mathbf{R}^{\emptyset}_{12}}^{T} & 0 \\ 0 & {\mathbf{R}^{\emptyset}_{12}}^{\dagger} \end{pmatrix}; \qquad \boldsymbol{\mathcal{A}}^{\emptyset} = \begin{pmatrix} \mathbf{R}^{\emptyset}_{22} & -\mathbf{I} \\ \mathbf{I} & -{\mathbf{R}^{\emptyset}_{22}}^{*} \end{pmatrix}. \tag{7.95b}$$

The Wick theorem can also be applied to ZME state. Likewise, it is possible to write the RDM in terms of correlation matrices and Majorana fermions of subsystem **1**. We can write the RDM as:

$$\rho^{\emptyset}_{\mathbf{1}}(\boldsymbol{\gamma}, \bar{\boldsymbol{\gamma}}) = [\det \frac{\mathbf{I} - \boldsymbol{\Gamma}^{\emptyset}_{\mathbf{1}}}{2}]^{\frac{1}{2}} e^{\frac{1}{4}\begin{pmatrix} \boldsymbol{\gamma} & \bar{\boldsymbol{\gamma}} \end{pmatrix} \ln \frac{\mathbf{I}+\boldsymbol{\Gamma}^{\emptyset}_{\mathbf{1}}}{\mathbf{I}-\boldsymbol{\Gamma}^{\emptyset}_{\mathbf{1}}} \begin{pmatrix} \boldsymbol{\gamma} \\ \bar{\boldsymbol{\gamma}} \end{pmatrix}}. \tag{7.96}$$

In the above expression, the matrix $\boldsymbol{\Gamma}^{\emptyset}_{\mathbf{1}}$ is defined in subsection 7.3.2, and the subscript stands for the correlation matrix for the subsystem.

7.4.4 Zero parity eigenstates

The zero parity eigenstates $|G_{\pm}\rangle$ are the cases where $\beta = \pm 1$. Using the results of (7.71) and (7.74), the RDM matrix in coherent basis and operator form for $|G_{\pm}\rangle$ are given by setting $\beta = \pm 1$.

7.4.5 Spin versus fermion representation

Although the previous considerations are advantageous numerically to study RDM's, we have to point out that the RDM for the spin representation and the fermionic representation (of the Hamiltonian) are not identical, necessarily. Correspondingly, the entanglement entropies could end up to be different. Based on the way of selecting the subsystem, RDM's (of spin and fermion representations) could be different or equal. This difference can be expected due to the non-local structure of the Jordan-Wigner transformation [124]. In general, we are interested in two scenarios for subsystem bipartition as demonstrated in the figure 5.

For start, if our desired state (like $|0\rangle$ and $|\emptyset\rangle$) is an eigenstate of parity operator, then RDM has equal form in spin and fermion representations for types (a) and (b) of subsystems in figure 5. Since the effect of the Jordan-Wigner strings disappears in

these cases. This statement is true for any boundary as long as boundary terms do not break the parity symmetry. If subsystem is not connected, then starting from fermionic representation, to obtain a spin correlation function (like $\langle\sigma_i^x\sigma_j^x\rangle$), one needs information about the string of sites between two blocks of subsystem in the fermionic picture, while, this is not necessary if one asks only for fermionic correlations.

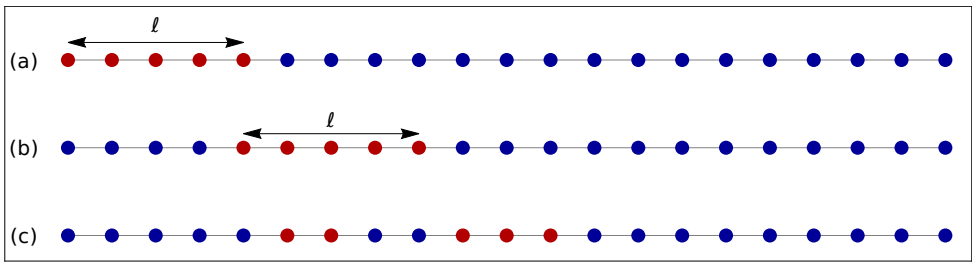


Figure 5 – The three subsystem block configurations we consider here. (a) a block of length ℓ starting from the boundary. (b) is a block of length ℓ at a distance from the boundary. The case (c) shows a disconnected subsystem which does not start from any of boundary points.

In the related case to our study, which we are dealing with an open boundary case and a state which does not respects the parity (like $|\beta\rangle$), then the relation between spin and fermion version of RDM is more peculiar. Essentially, the string of σ^z's from Jordan-Wigner transformation would break off the correspondence between spins and fermions for a subsystem separated from the boundary, similar to (b) in figure 5. It is an anomaly of parity broken state that the RDM of any interval starting from the boundary is the same for spins and fermions. While not starting from one of the boundaries of the chain, other techniques should be used to find the RDM of spin representation [135]. The arguments that are presented in this part can be summarized in the table 2.

Tabela 2 – A handy representation of the statements in the section 7.4.5. In the below, ρ_{spin} stands for the RDM in the spin representation and ρ_{fermion} is the RDM in the fermionic representation of the Hamiltonian. The subsystem types are demonstrated in figure 5. In addition, we have assumed the restriction on $\beta \neq 0, \infty$.

State \ Subsystem	type (a)	type (b)	type (c)
$\|0\rangle$, $\|\emptyset\rangle$	$\rho_{\text{spin}} = \rho_{\text{fermion}}$	$\rho_{\text{spin}} = \rho_{\text{fermion}}$	$\rho_{\text{spin}} \neq \rho_{\text{fermion}}$
$\|\beta\rangle$	$\rho_{\text{spin}} = \rho_{\text{fermion}}$	$\rho_{\text{spin}} \neq \rho_{\text{fermion}}$	$\rho_{\text{spin}} \neq \rho_{\text{fermion}}$

7.5 Entanglement Entropy

Given the reduced density matrix ρ_A describing knowledge of the state of a subsystem A, the Rényi entanglement entropy is given by:

$$S_n(A) = \frac{1}{1-n}\log(\text{tr}_A\rho_A^n). \tag{7.97}$$

The Rényi entanglement entropy can be seen as the generalized version of von Neumann entanglement measure. In the limit $\alpha \to 1$, Rényi EE produces the Von Neumann EE (S_{vN}),

$$S_{vN}(A) = -\mathrm{tr}_A[\rho_A \log \rho_A]. \tag{7.98}$$

The difficulty of calculation of the entanglement grows exponentially with size of the subsystem. One can find a basis which RDM is diagonal, however, it would still be computationally disadvantageous.

It is possible to have special structure for the RDM to simplify the entanglement calculation. For instance having a Gaussian form for RDM simplifies the calculation, or being able to write the RDM in terms of correlation matrices. In the rest of this section, we first present the result of entanglement for the vacuum state and the ZME state which are basically the results in [65, 67, 68, 69]. We are going to give the entanglement in terms of the eigenvalues of the correlation matrices and Gaussian form of the RDM. Next, we will discuss the entanglement calculation for a general parity broken state such as $|\beta\rangle$ and the limiting cases of $|G_\pm\rangle$ which are new.

7.5.1 Vacuum and ZME state

Since the Wick theorem can be applied to the vacuum state we were able to write the RDM as (7.87). Using the equations (7.87) and (7.97), we can trace the RDM and write the Rényi entanglement for this state as

$$S_n^0(A) = \frac{1}{1-n} \log \left(\mathrm{C}^\alpha \det\left[\mathbf{I} + e^{n\boldsymbol{\mathcal{M}}}\right]^{\frac{1}{2}} \right), \tag{7.99}$$

where the constant C is given by

$$\mathrm{C} = \frac{\sqrt{\det\left[\mathbf{I}+\mathbf{R}_{22}{}^\dagger \mathbf{R}_{22}\right]}}{\sqrt{\det\left[\mathbf{I}+\mathbf{R}^\dagger \mathbf{R}\right]}} e^{\frac{1}{2}\mathrm{tr}\ln(\frac{1}{2}\boldsymbol{\Omega}_{12}-\frac{1}{2}\boldsymbol{\Omega}_{21}^T)}. \tag{7.100}$$

The matrices $\boldsymbol{\mathcal{M}}$ and $\boldsymbol{\Omega}$ are already defined in (7.88). This relation is computationally favorable, since all we need to calculate is a determinant.

As it was written in section 7.4.2, we could have also express the RDM in terms of correlation matrices of Majorana fermions (7.89). Therefore, it is possible to find the entanglement in terms of the correlation matrix $\boldsymbol{\Gamma}^0$ (of the vacuum state) for the subsystem A. Therefore, using the RDM (7.89) and the trace formula for Gaussian function of fermions, the Rényi EE is given by

$$S_n^0(A) = \frac{1}{2(1-n)} \log\det\left[(\frac{1+\boldsymbol{\Gamma}_A^0}{2})^n + (\frac{1-\boldsymbol{\Gamma}_A^0}{2})^n\right] = \frac{1}{(1-n)} \sum_j \log\left[(\frac{1+\nu_j^0}{2})^n + (\frac{1-\nu_j^0}{2})^n\right] \tag{7.101}$$

where the set of $\{\pm\nu_k\}$ are the eigenvalues of $\mathbf{\Gamma}^0_A$ for the subsystem A. The above relation is favorable because it is straightforward to find the correlation matrix for states that obeys Wick theorem.

The entanglement for the ZME state can have a similar form. For instance, in subsection (7.4.3), it was mentioned that through some canonical transformations it is possible to write the RDM in Gaussian form (7.94). Similar to previous state, using the Gaussian form of RDM and tracing that, we can get the Rényi entanglement for subsystem A same as (7.99) but we have to use $\mathbf{R}^{\emptyset}$ instead of $\mathbf{R}^0$. On the other hand, the Wick theorem can be applied to the ZME state. Hence, it is possible to relate the EE to the correlation matrices, similar to (7.101). We only need to use the $\mathbf{\Gamma}^{\emptyset}_A$ given in section 7.3.2.

Based on the form of $\mathbf{\Gamma}^{\emptyset}_A$ and $\mathbf{\Gamma}^0_A$, one can deduce that for any subsystem A which does not include the last lattice point $L+1$, they have equal set of eigenvalues ($\{\nu^0\}=\{\nu^{\emptyset}\}$). It also means that the entanglement S^0_α and $S^{\emptyset}_\alpha$ are equal. It means that the states $|0\rangle$ and $|\emptyset\rangle$ have the same entanglement properties for any given model ($\mathbf{A}$ and $\mathbf{B}$ matrices which depend on the model).

7.5.2 General β-parity broken state

Unlike the vacuum and ZME states, there are not many computationally easy methods to study the entanglement entropy for a state such as $|\beta\rangle$. Namely, we can not use the correlation matrix blindly for this state. In this subsection, we first focus on a computationally favorable method to study the EE for such state. Then, we offer a relation for special type of bipartition which relies on correlation matrix. For start, when $n\in\mathbb{N}$ we can use Berezin integrations to find the $\rho_A^{\beta\,n}$. The steps of calculation are written in appendix D. The Rényi entanglement entropy for $n=2$ is given by:

$$\begin{aligned}\mathrm{tr}(\rho_A^{\beta\,2}) =&\mathcal{C}^{\beta^2}\mathrm{Pf}[\boldsymbol{\mathcal{B}}]\Big\{\Big(\frac{1}{|\beta|^2}+\mathrm{Pf}[\boldsymbol{\mathcal{W}}]\Big)^2+\mathrm{Pf}[\boldsymbol{\mathcal{W}}]\Big(\mathbb{C}\boldsymbol{\mathcal{B}}^{-T}\mathbb{C}^T|_{1,2}+\mathbb{C}\boldsymbol{\mathcal{B}}^{-T}\mathbb{C}^T|_{3,4}\Big)\\ &-\frac{\mathbb{C}\boldsymbol{\mathcal{B}}^{-T}\mathbb{C}^T|_{2,4}}{\beta^2}-\frac{\mathbb{C}\boldsymbol{\mathcal{B}}^{-T}\mathbb{C}^T|_{1,3}}{\beta^{*2}}+\frac{1}{|\beta|^2}\Big(\mathbb{C}\boldsymbol{\mathcal{B}}^{-T}\mathbb{C}^T|_{1,2}+\mathbb{C}\boldsymbol{\mathcal{B}}^{-T}\mathbb{C}^T|_{3,4}-\mathbb{C}\boldsymbol{\mathcal{B}}^{-T}\mathbb{C}^T|_{2,3}\\ &-\mathbb{C}\boldsymbol{\mathcal{B}}^{-T}\mathbb{C}^T|_{1,4}\Big)+\mathrm{Pf}[\mathbb{C}.\boldsymbol{\mathcal{B}}^{-T}.\mathbb{C}^T]\Big\}.\end{aligned} \tag{7.102}$$

Where,

$$\boldsymbol{\mathcal{B}}=\begin{pmatrix}\mathbf{\Omega}_{11} & \mathbf{0} & -\mathbf{\Omega}_{12} & \mathbf{I}\\ \mathbf{0} & \mathbf{\Omega}_{11} & \mathbf{I} & \mathbf{\Omega}_{12}\\ -\mathbf{\Omega}_{21} & -\mathbf{I} & \mathbf{\Omega}_{22} & \mathbf{0}\\ -\mathbf{I} & \mathbf{\Omega}_{21} & \mathbf{0} & \mathbf{\Omega}_{22}\end{pmatrix},\qquad \mathbb{C}=\begin{pmatrix}-\boldsymbol{\mathcal{L}}_1 & \mathbf{0} & \boldsymbol{\mathcal{L}}_2 & \mathbf{0}\\ -\boldsymbol{\mathcal{L}}_3 & \mathbf{0} & \boldsymbol{\mathcal{L}}_4 & \mathbf{0}\\ \mathbf{0} & \boldsymbol{\mathcal{L}}_1 & \mathbf{0} & \boldsymbol{\mathcal{L}}_2\\ \mathbf{0} & \boldsymbol{\mathcal{L}}_3 & \mathbf{0} & \boldsymbol{\mathcal{L}}_4\end{pmatrix}. \tag{7.103}$$

The $\mathbf{\Omega}$ and $\boldsymbol{\mathcal{L}}$ are given by (7.72). Also, the notation $\mathbb{X}|_{r,s}$ stand for the element of the matrix $\mathbb{X}$ at the position (r, s). The above expression can be used for any bipartition of the system. However, we are restricted to the $n = 2$. From section 7.3.3, we expect to see no β-dependence in the entanglement entropy when the subsystem does not contain boundary points [124]. Despite that, the entanglement content would not be the same from spin perspective to the fermion one. For the case of general parity broken state, if subsystem is not a connected bipartition starting from boundary, then spin entanglement and fermion entanglement do not agree.

In section 7.4.1, we proved that it is possible to have an ansatz to write the RDM in the diagonal form of (7.80). Using this form of RDM one can write the Rényi EE as:

$$S_n^\beta(A) = \frac{1}{1-n}\sum_{j=1}^{l}\log\Big((\frac{1+\nu_j}{2})^n + (\frac{1-\nu_j}{2})^n\Big) + \frac{1}{1-n}\log[(\tfrac{1}{2}+\mathrm{f}_\beta)^n + (\tfrac{1}{2}-\mathrm{f}_\beta)^n], \quad (7.104)$$

where $\mathrm{f}_\beta = \frac{\mathrm{Re}[\beta]}{1+|\beta|^2}$, and it is the eigenvalue of the zeroth part of RDM (7.80). In the above ν_j's are the eigenvalues of correlation matrix $\mathbf{\Gamma}^\beta$. The formula above simplifies the entanglement studies, however, it is valid for a certain type of the subsystems. The set A should be connected subsystem of the system containing the site 0 (first site). Otherwise, we would not be able to get entanglement from correlations of the system.

It is crucial to mention that form of correlation $\mathbf{\Gamma}^\beta$, in (7.65) and (7.66), indicates that the eigenvalues of $\mathbf{\Gamma}_A^\beta$ for any subsystem $0 \in A$ and $L+1 \notin A$ are the same as $\mathbf{\Gamma}_A^0$. This statement means that there is a relation between entanglements $S_n^0(A)$, $S_n^\emptyset(A)$ and $S_n^\beta(A)$ (only when $n \neq 1$);

$$S_n^0(A) = S_n^\emptyset(A) = S_n^\beta(A) + \frac{1}{1-n}\log[\frac{2^{1-n}}{(\frac{1}{2}+\mathrm{f}_\beta)^n + (\frac{1}{2}-\mathrm{f}_\beta)^n}]. \quad (7.105)$$

7.5.3 Zero parity eigenstates

The Rényi entanglement for states $|G_\pm\rangle$ can be computed in different ways. One can use the (7.102) in the limit $\beta \to 1$. However, similar to section 7.4.4, it is possible to have an ansatz to write the RDM in the diagonal form of (7.80). Using this form of RDM one can write the Rényi EE as [156]:

$$S_n^\pm(A) = \frac{1}{1-n}\sum_{j=0}^{l}\log\Big((\frac{1+\nu_j}{2})^n + (\frac{1-\nu_j}{2})^n\Big) - \log 2. \quad (7.106)$$

In the above $\nu^\pm$ are the eigenvalues of correlation matrix $\mathbf{\Gamma}^\pm$. The above formula simplifies the entanglement studies, however, it is valid for a certain type of the subsystems. The set A should be connected subsystem of the system containing the site 0 (first site). Otherwise, we would not be able to get entanglement from correlations of the system.

It is crucial to mention that form of correlation $\mathbf{\Gamma}^\pm$, in (7.65) and (7.66), indicates that the eigenvalues of $\mathbf{\Gamma}_A^\pm$ for any subsystem $0 \in A$ and $L+1 \notin A$ are the same as $\mathbf{\Gamma}_A^0$.

This statement means that there is a relation between entanglements $S_n^0(A)$, $S_n^\emptyset(A)$ and $S_n^\pm(A)$;

$$S_n^0(A) = S_n^\emptyset(A) = S_n^\pm(A) + \log 2. \tag{7.107}$$

And it is correct for any valid choices of **A** and **B** matrices. In fact, one can extend this argument to any excited state created from $|0\rangle$, $|\emptyset\rangle$ and $|G_\pm\rangle$ with excitation of same modes, as in

$$|\psi\rangle = \prod_{k_j\in\mathbb{E}} \eta_{k_j}^\dagger |0\rangle\,, \qquad |\phi\rangle = \prod_{k_j\in\mathbb{E}} \eta_{k_j}^\dagger |\emptyset\rangle\,, \qquad |\chi_\pm\rangle = \prod_{k_j\in\mathbb{E}} \eta_{k_j}^\dagger |G_\pm\rangle\,.$$

where set $\mathbb{E}$ does not contain mode zero. The general form of correlations for states above can be found in appendix D. Based on the results of that appendix, we conclude that

$$S_n^\psi(A) = S_n^\phi(A) = S_n^{\chi_\pm}(A) + \log 2. \tag{7.108}$$

7.6 Physical interpretation of the parity-broken state

In this section, we give a simple interpretation of the $|\beta\rangle$ state which helps to understand some simple cases of the results that we presented so far. This sate can be written as follows:

$$|\beta\rangle = \frac{1}{\sqrt{2(1+|\beta|^2)}}\Big((1+\beta)\,|G_+\rangle + (1-\beta)\,|G_-\rangle\Big). \tag{7.109}$$

In the spin representation the above state can be written in an interesting form. Consider $\delta_+ = 1$ then we can write

$$|\beta\rangle = \frac{1}{\sqrt{2(1+|\beta|^2)}}\Big((1+\beta)\,|+\rangle_0\,|\phi_{++}\rangle\,|+\rangle_{L+1} + (1-\beta)\,|-\rangle_0\,|\phi_{--}\rangle\,|-\rangle_{L+1}\Big), \tag{7.110}$$

where $|\phi_{--}\rangle$ and $|\phi_{++}\rangle$ are normalized states. The above form suggests that the whole system can be considered as two qubit with one qubit at site 0 $(L+1)$ and the other the rest of the system. Interestingly, the entanglement structure of these three parts is independent of the size of the system and one can easily calculate for example the entanglement of the site 0 $(L+1)$ with the rest, i.e. $S_n(0)$ $(S_n(L+1))$;

$$S_n(0) = S_n(L+1) = \frac{1}{1-n}\log[(\tfrac{1}{2}+\mathrm{f}_\beta)^n + (\tfrac{1}{2}-\mathrm{f}_\beta)^n], \tag{7.111}$$

which is consistent with the equation (7.104). We note that one can generalize the above argument for all the $|\beta\rangle$ states that can be made out of the eigenstates. The extension to $\delta_+ = -1$ is straightforward. Finally, there is one extra piece that one can add to this story by considering the following mixed state:

$$\rho^\beta = \frac{1}{2(1+|\beta|^2)}\Big(|1+\beta|^2\,|G_+\rangle\langle G_+| + |1-\beta|^2\,|G_-\rangle\langle G_-|\Big). \tag{7.112}$$

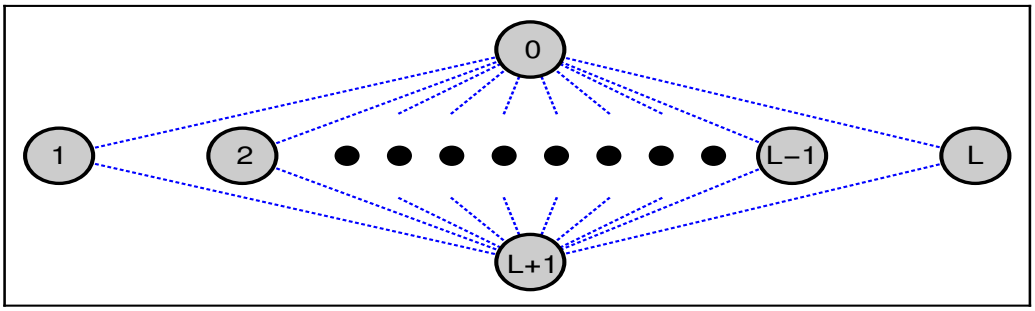


Figure 6 – In this figure the type of interaction among fermions at different sites, for $\mathbf{A} = \mathbf{B} = 0$ is demonstrated. As one can see, there is no particle hoping among sites 1 to L and the only allowed hoping is from sites 0 or $L + 1$ with the rest of sites.

One can easily show that the reduced density matrix of the above state is exactly equal to the reduced density matrix of the $|\beta\rangle$ state which is guarantied because of the especial form of the state. This makes the preparation of states with the desired reduced density matrix very easy. However, it is clear that in the mixed state scenario the von Neumann entropy does not have entanglement interpretation anymore.

7.7 Examples

In this section, we provide a couple of examples to show how the general results that we derived can be applied in specific cases. The first example which we are able to do the entire calculation analytically is the Hamiltonian (7.5) with $\boldsymbol{A} = \boldsymbol{B} = 0$. There are a few good reasons to study this Hamiltonian. First of all, for this Hamiltonian one can follow all the calculations analytically and show the validity of all the presented results. Second, it is a Hamiltonian that can be used to diagonalize a Hermitian Hamiltonian with linear creation and annihilation operators which makes it worth studying. Finally interestingly the entanglement structure that emerges from this Hamiltonian is entirely universal. In other words the general Hamiltonians with generic parameters end up to have similar entanglement structure. This is shown in the example of XY chain with arbitrary boundary magnetic fields which is the second example of this section. The boundary conformal entanglement entropy at the critical point in this case has been studied already in [156], however, here we are more concentrated on general aspects of entanglement with respect to the β parameter and boundary magnetic fields.

7.7.1 $\boldsymbol{A} = \boldsymbol{B} = 0$

We are going to focus on the entanglement properties here of the case where the $\mathbf{A}$ and $\mathbf{B}$ matrices are zero. The coupling of fermions in the system has been demonstrated in figure 6. A detailed study is presented in Appendix D for diagonalization and correlations of this special case.

For the vacuum state and ZME state, which Wick theorem is applicable as it was stated in section 7.5.1, we can relate the Rényi entanglement to the eigenvalues of correlation matrix $\mathbf{\Gamma}$ introduced in (3.2). In a special type of system bipartition, we could also use the $\mathbf{\Gamma}^{\pm}$ to find entanglement for the $|G_{\pm}\rangle$ case. For any connected subsystem which contains the site 0 (or site $L+1$), the (positive valued) eigenvalues of correlation matrices $\mathbf{\Gamma}^{0}$, $\mathbf{\Gamma}^{\emptyset}$ and $\mathbf{\Gamma}^{\pm}$ are given by the set:

$$\{\nu\} = \begin{cases} \{0, \sqrt{1-\frac{(\sum_{j=1}^{\ell}|\alpha_j|^2)(\sum_{j=\ell+1}^{L}|\alpha_j|^2)}{(\sum_{j=1}^{L}|\alpha_j|^2)^2}}, 1, \cdots, 1\} & \ell \leq L, \\ \{1, \cdots\cdots, 1\} & \ell = L+1. \end{cases} \tag{7.113}$$

The fact that we get the same eigenvalues for each of the states above was explained in section 7.5. Based on the form of correlation matrices similar (up to a zero eigenvalue) eigenvalues was expected. Using the eigenvalues above the entanglement will be given by ($\ell \leq L$)

$$\begin{aligned} S_n^0(\ell) &= S_n^{\emptyset}(\ell) = \frac{1}{1-n}\log\Bigg((\frac{1}{2}+\frac{1}{2}\sqrt{1-\frac{(\sum_{j=1}^{\ell}|\alpha_j|^2)(\sum_{j=\ell+1}^{L}|\alpha_j|^2)}{(\sum_{j=1}^{L}|\alpha_j|^2)^2}})^n \\ &\quad +(\frac{1}{2}-\frac{1}{2}\sqrt{1-\frac{(\sum_{j=1}^{\ell}|\alpha_j|^2)(\sum_{j=\ell+1}^{L}|\alpha_j|^2)}{(\sum_{j=1}^{L}|\alpha_j|^2)^2}})^n\Bigg) + \log 2, \end{aligned} \tag{7.114}$$

$$S_n^{\pm}(\ell) = S_n^0(\ell) - \log 2. \tag{7.115}$$

In case where all the α_i's are constant, we would get

$$S_n^0(\ell) = \frac{1}{1-n}\log\left((\tfrac{1}{2}+\tfrac{1}{2}\sqrt{\tfrac{L^2-\ell L+\ell^2}{L^2}})^n + (\tfrac{1}{2}-\tfrac{1}{2}\sqrt{\tfrac{L^2-\ell L+\ell^2}{L^2}})^n\right) + \log 2, \tag{7.116}$$

In the thermodynamic limit ($L \to \infty$), we simply get $S_n^0(\ell) = S_n^{\emptyset}(\ell) = \log 2$ and $S_n^{\pm}(\ell) = 0$.

For any connected bipartition of system with length ℓ which does not contain the 0^{th} and $L+1^{\text{th}}$ sites, eigenvalues of $\mathbf{\Gamma}^0$ and $\mathbf{\Gamma}^{\emptyset}$ are given by

$$\{\nu\} = \begin{cases} \{\frac{\sum_{k=\ell+1}^{L}|\alpha_k|^2}{(\sum_{k=1}^{L}|\alpha_k|^2)^2}, 1, 1, \cdots, 1\}; & \ell \leq L, \\ \{0, 1, 1, \cdots, 1\}; & \ell = L+1. \end{cases} \tag{7.117}$$

With this type of bipartition for the system, then the correlation matrix can be used to calculate the entanglement for states $|0\rangle$ and $|\emptyset\rangle$. While for the state $|G_{\pm}\rangle$ we can not, despite the fact that the $\mathbf{\Gamma}^{\pm}$ has the same eigenvalues.

In the case of general β-state, and when $\alpha_i \in \mathbb{R}$, the von Neumann entanglement will be:

$$\begin{aligned} S_{vN}^{\beta}(A) = &-\tfrac{1}{2}\log\left[(\frac{1}{4}-\mathrm{f}_\beta)\frac{\Sigma_l\Sigma_{L-l}}{4\Sigma_L^2}\right] - \mathrm{f}_\beta\log\left(\frac{1+2\mathrm{f}_\beta}{1-2\mathrm{f}_\beta}\right) \\ &- \tfrac{\sqrt{\Sigma_L^2-\Sigma_l\Sigma_L+\Sigma_l^2}}{2\Sigma_L}\log\left[\frac{\Sigma_L+\sqrt{\Sigma_L^2-\Sigma_l\Sigma_L+\Sigma_l^2}}{\Sigma_L-\sqrt{\Sigma_L^2-\Sigma_l\Sigma_L+\Sigma_l^2}}\right]. \end{aligned} \tag{7.118}$$

Where in the above $\Sigma_l = \sum_{j=1}^{l} \alpha_j^2$ and $\mathrm{f}_\beta = \frac{\mathrm{Re}[\beta]}{1+|\beta|^2}$. It is particularly interesting to see the behavior of entanglement with respect to the β. As it was mentioned previously, parameter β can be thought as a parameter which breaks the parity continuously. In figure 7, we have demonstrated a typical behavior of EE for different values of β in complex plain when all α_i's are real constants. As you can see, for real values of β, the entanglement is maximum for $\beta = 0, \infty$ and minimum for $\beta = \pm 1$, which the first one corresponds to vacuum and ZME state and second one is the $|G_\pm\rangle$. On the other hand, for the purely imaginary β, entanglement is constant and equal to $S_2^0(l)$ for any value of β which is not a trivial observation.

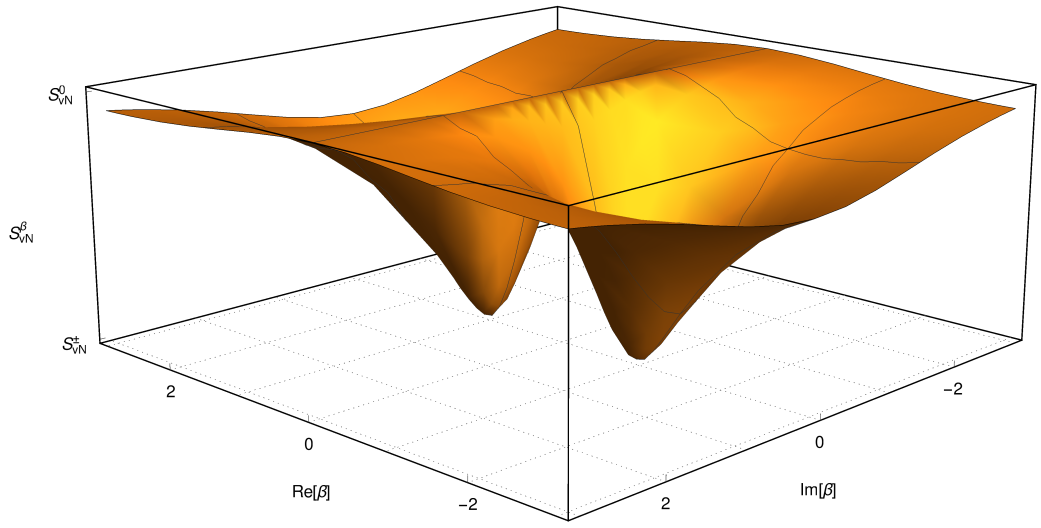


Figure 7 – Plot of von Neumann entanglement entropy with respect to β. We already expected that the entanglement to be minimum for the case of $\beta = \pm 1$ which is apparent in the figure. In the case where β is purely imaginary, we notice that the EE is again maximum and would not change. This figure is valid for a connected subsystem starting from site 0, for a general set of couplings in the Hamiltonian and size of the full system and subsystem.

7.7.2 Modified **XY** chain with boundary magnetic field

In this section, we consider the modified transverse field XY chain with arbitrary direction of the boundary magnetic field. We are interested in the following XY Hamiltonian[156] with open boundary conditions

$$\begin{aligned}\mathcal{H}^{XY} =& J\sum_{i=1}^{L-1}\Big[\frac{1+\gamma}{4}\sigma_i^x\sigma_{i+1}^x + \frac{1-\gamma}{4}\sigma_i^y\sigma_{i+1}^y\Big] - \frac{h}{2}\sum_{i=1}^{L}\sigma_i^z \\ &+ \frac{1}{2}\Big(b_{1,x}\sigma_0^x\sigma_1^x + b_{1,y}\sigma_0^x\sigma_1^y + b_{1,z}\sigma_1^z + b_{L,x}\sigma_L^x\sigma_{L+1}^x + b_{L,y}\sigma_L^y\sigma_{L+1}^x + b_{L,z}\sigma_L^z\Big)\end{aligned} \tag{7.119}$$

where $\overrightarrow{b_1} = (b_1\sin\theta_1\cos\varphi_1, b_1\sin\theta_1\sin\varphi_1, b_1\cos\theta_1)$ and $\overrightarrow{b_L} = (b_L\sin\theta_1\cos\varphi_1, b_L\sin\theta_1\sin\varphi_1, b_L\cos\theta_1$ are constant vectors. Form of $\mathcal{H}^{XY}$ suggests that we can diagonalize and find the eigenstates analytically. Using the Jordan-Wigner transformation

$$c_l^\dagger = \prod_{j=0}^{l-1}\sigma_j^z\sigma_l^+, \tag{7.120}$$

where $\sigma_n^{\pm} = \frac{\sigma_n^x \pm i\sigma_n^y}{2}$, we can map the Hamiltonian (7.119) to the free fermion Hamiltonian (7.8), with properly chosen matrices $\mathbf{M}$ (see appendix D for a demonstration of this matrix). The diagonalization process has been explained in details in section 7.2.3. The above Hamiltonian is related to an XY chain with boundary magnetic fields as:

$$H^{XY} = J\sum_{i=1}^{L-1}\Big[\frac{1+\gamma}{4}\sigma_i^x\sigma_{i+1}^x + \frac{1-\gamma}{4}\sigma_i^y\sigma_{i+1}^y\Big] - \frac{h}{2}\sum_{i=1}^{L}\sigma_i^z + \frac{1}{2}(\overrightarrow{b}_1.\overrightarrow{\sigma}_1 + \overrightarrow{b}_L.\overrightarrow{\sigma}_L). \quad (7.121)$$

In the above expression, we can think of $\overrightarrow{b}_1$ and $\overrightarrow{b}_L$ as magnetic fields at boundaries of our spin chain. If we add two auxiliary spins at positions 0 and $L+1$, if they can only interact with the x component of spins at position 1 and L, then we get (7.119). It is apparent that $\mathcal{H}^{XY}$ commutes with σ_0^x and σ_{L+1}^x. Due to this fact it is possible to divide the Hilbert space of $\mathcal{H}^{XY}$ in four distinct sectors, labeled by the eigenvalues of σ_0^x and σ_{L+1}^x. Therefore, the eigenstates of Hamiltonian (7.121) would be found in one of these sectors. This procedure has been explained in section 7.2.6.

7.7.2.1 Determination of BMF Hamiltonian eigenstates

The eigenstates of Hamiltonian (7.121) can be found with a correct projection in the Hilbert space of (7.119), which was mentioned in the section (7.2.6). Here, we focus on the XY-chain case and present (apparent) patterns to find the ground state of (7.121). Based on results of (7.45) and (7.46), one can identify the ground state of BMF spin chain in $|G_+\rangle$ or $\eta_{min}^\dagger|G_-\rangle$[4] by finding the δ_+. Numerical investigations suggests that the value of δ_+ does not depend on the parameters such as γ, h (fixing $J=-1$) and strength of the magnetic field at boundaries. The size of the full system however changes the value of δ_+; For equal directions of boundary fields ($\overrightarrow{b}_1$ and $\overrightarrow{b}_L$) we get:

$$\begin{cases}\delta_+ = -1 & L \text{ even},\\ \delta_+ = +1 & L \text{ odd}.\end{cases} \quad (7.122)$$

Nonetheless, the change in the directions of BMF's at ends of the chain can affect the value of δ_+. Figure 8 shows the δ_+ with respect to the change in the azimuthal and polar angle of direction of the magnetic field at boundaries. If one eliminates the BMF at one end of the system (either by putting $\theta_1 = 0, \pi$ or $b_1 = 0$), then changing the direction or strength of BMF at the other end would not affect the δ_+ outcome.

To be able to use the relation (7.74), one need to have the unitary transformation $\mathbf{U}$, which diagonalizes the Hamiltonian, in the form given by (7.15). Necessary condition is to make sure that eigenstates of $\mathbf{M}$ corresponding to zero modes are written correctly, they are orthogonal and satisfy the (2.47). We have already introduced the zero mode of the system in section 7.2.2, which explains the 2-fold degeneracy of the ground state.

[4] $\eta_{min}^\dagger$ is the creation operator for the mode with the smallest non-zero energy.

However, based on some values of coupling parameters (such as uniform external magnetic field or direction of boundary fields) there could arise more zero modes in the spectrum of $\mathbf{M}$ matrix. For instance, when $\gamma = 1$ and $\varphi_1, \varphi_L = \frac{\pi}{2}$ (and general bulk and boundary magnetic fields h, $\overrightarrow{b}_1$, $\overrightarrow{b}_L$), we would have extra zero mode and more degeneracy. For this values, the extra zero modes eigenvectors of $\mathbf{M}$ would be (besides (7.12))

$$\left|u_0^3\right\rangle = \frac{1}{\sqrt{4+2\zeta_1^2+2\zeta_L^2}} \begin{pmatrix} -i\zeta_1 \\ 1 \\ 0 \\ \vdots \\ 0 \\ -1 \\ i\zeta_L \\ i\zeta_1 \\ 1 \\ 0 \\ \vdots \\ 0 \\ 1 \\ i\zeta_L \end{pmatrix}, \qquad \left|u_0^4\right\rangle = \frac{1}{\sqrt{4+2\zeta_1^2+2\zeta_L^2}} \begin{pmatrix} -i\zeta_1 \\ 1 \\ 0 \\ \vdots \\ 0 \\ 1 \\ -i\zeta_L \\ i\zeta_1 \\ 1 \\ 0 \\ \vdots \\ 0 \\ -1 \\ -i\zeta_L \end{pmatrix}; \tag{7.123}$$

where $\zeta_{1,L} = \frac{h - b_{1,L}\cos\theta_{1,L}}{b_{1,L}\sin\theta_{1,L}}$. This is an exact zero mode which comes from the fact that BMF's does not have any component in the x-direction. In general, there could be more zero modes for large sizes. It does not seem easy to identify analytically all the points where we face degeneracy more than the two mentioned. To study entanglement, one should be careful with the zero modes. As an example, numerical investigations suggests that for $L >> 1$, we would expect one more zero mode for $h > 1$ and independent from BMF values.

7.7.2.2 Entanglement studies

Regarding the entanglement, we have looked into the entanglement properties of parity broken state $|\beta\rangle$. For instance, the behavior of von Neumann entanglement entropy is plotted with respect to the parameter β in the figure 9 for fixed and equal angles of boundary fields. Looking to the discussion of section 7.5.2, the entanglement entropy obeys the relation

$$S_n^0(A) = S_n^{\emptyset}(A) = S_n^{\beta}(A) + \frac{1}{1-n}\log[\frac{2^{1-n}}{(\frac{1}{2}+\mathrm{f}_\beta)^n + (\frac{1}{2}-\mathrm{f}_\beta)^n}], \qquad \mathrm{f}_\beta = \frac{\mathrm{Re}[\beta]}{1+|\beta|^2}. \tag{7.124}$$

Since the relation above is general and does not depend on parameters of the model, it is expected to see the same behavior of entanglement entropy with the change in the β as in figure 7.

For most parts of this subsection, we are interested in case where the boundary magnetic fields are the same in both edges, i. e., $\vec{b}_1 = \vec{b}_L$. Another compelling observation would be the effect of the boundary field direction (same in both ends) on the entanglement of a particular state such as $|G_+\rangle$. Results have been demonstrated in figure 10. For specific angles of BMF in the xy-plane, we observe a huge change in the value of entanglement entropy. For the small magnetic field ($h < J$ as in figure 10a), there are two degenerate ground states for BMF Ising model: one can write $\frac{1}{2}(|\rightarrow\rightarrow\cdots\rightarrow\rangle + |\leftarrow\leftarrow\cdots\leftarrow\rangle)$ as the ground state. When $\varphi \approx 0$, the first spin prefers $|\rightarrow\rangle$ over the other possibility, $|\leftarrow\rangle$, which lowers the boundary entanglement [5] . As $\varphi \to \frac{\pi}{2}, \frac{3\pi}{2}$, both possible state of x-spin for the first spin would be equally probable, since the boundary magnetic field aligns the first spin in the (positive or negative) y direction. This would result in increase in entanglement. As the angle θ increases, the intensity of BMF interaction $\vec{b}_1.\vec{S}_1$ opposes the uniform magnetic field h in the system. So, we would expect smaller jumps in the entanglement for bigger θ.

In the large magnetic fields ($h > J$ as in figure 10c or the paramagnetic state) the ground state is not degenerate, being all spins almost aligned in the direction of h. When BMF in the xy-plan is small ($\theta \approx 0, \pi$), entanglement would not change much by change in φ. Although almost constant, entanglement is a bit higher for small $\theta \sim 0$ rather than $\theta \sim \pi$. As the intensity of BMF in xy-plan increases (for example $\theta = \frac{\pi}{4}$), first few spins at the beginning of the chain would get out of all parallel positioning and the entanglement changes with the angle of φ.

Conclusions

In this chapter, we investigated a generic quantum spin chain Hamiltonian with arbitrary boundary magnetic fields. As far as the bulk Hamiltonian can be mapped to free fermions even though the boundary terms are not quadratic with respect to free fermions we were able to diagonalize the Hamiltonian exactly. This was done using two ancillary extra sites and later projection of the eigenstates. The extended Hamiltonian was studied in depth and many properties of the Hamiltonian was studied including eigenstates in configuration bases, the correlation function of eigenstates and the reduced density matrix. The extended Hamiltonian always has at least one zero mode which guaranties the presence of degeneracy. To get the eigenstates of the original spin chain one needs to go to the sector in which the parity number symmetry is broken. We studied comprehensively these eigenstates and found the correlation functions, reduced density matrix and the entanglement entropy.

[5] Size of the subsystem has considered to be small so effect of boundary entanglement be more apparent

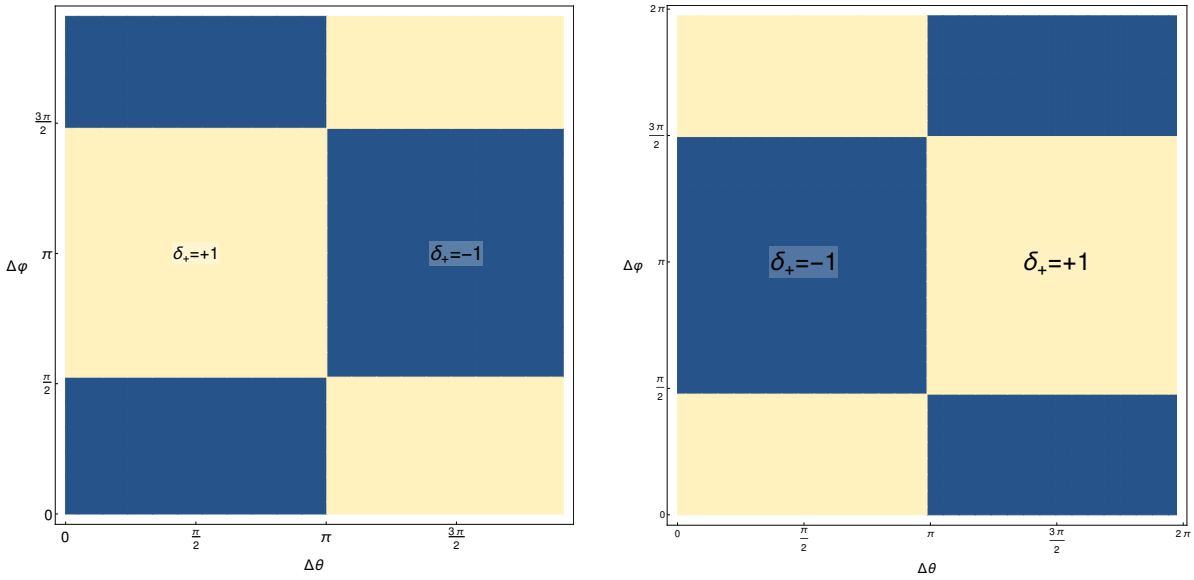


Figure 8 – Different values of δ_+ for difference in the directions of boundary fields $\vec{b_1} = (\sin\theta_1\cos\varphi_1, \sin\theta_1\sin\varphi_1, \cos\theta_1)$ and $\vec{b_L} = (\sin\theta_L\cos\varphi_L, \sin\theta_L\sin\varphi_L, \cos\theta_L)$. We have defined $\Delta\varphi = \varphi_L - \varphi_1$ and $\Delta\theta = \theta_L - \theta_1$. The direction of boundary field at the first site is fixed by $\theta_1 = \varphi_1 = \frac{\pi}{200}$ and we change the angles at end point of the chain. On the right, we have $L = 9$ and left hand side corresponds to $L = 10$. Rest of the parameters are: $J = -1$, $\gamma = 1/2$ and $h = 0.518$.

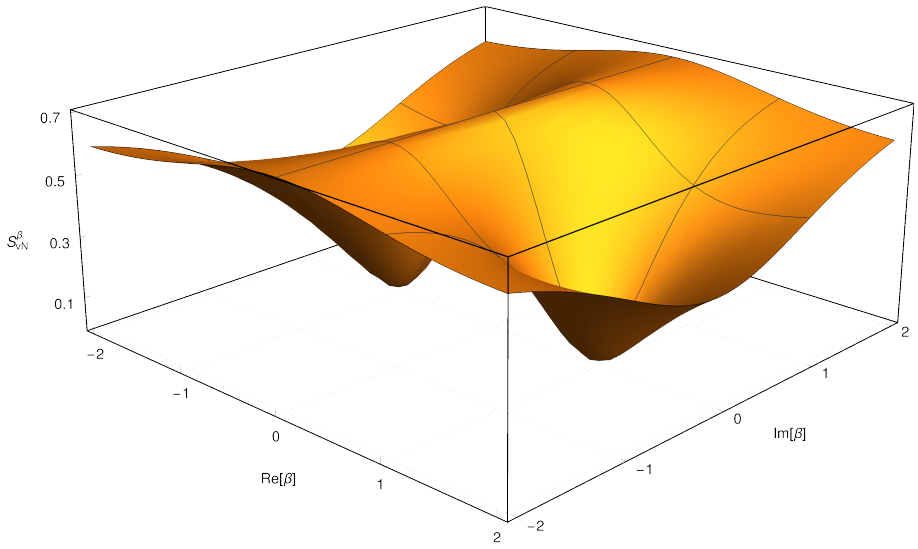
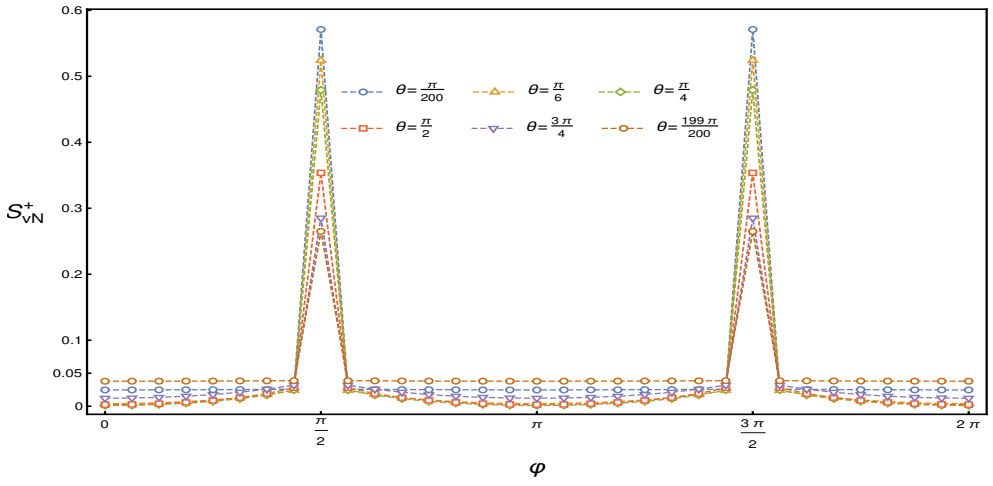
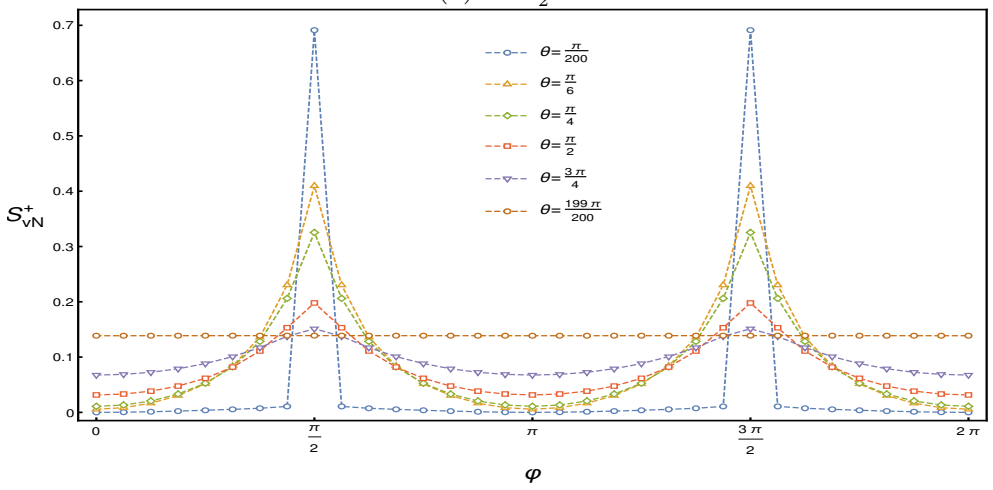


Figure 9 – In above, the typical behavior of von Neumann entropy with respect to parameter β is plotted for a subsystem of length ℓ starting from boundary of the chain. Size of the full system is $L = 30$ and subsystem is $l = 14$. Rest of the parameters are: $J = \gamma = 1$, $h = \frac{1}{2}$, $b_{L,x,y} = 1$, $b_{1,x,y} = 1$ and $b_{1,L,z} = 0$.

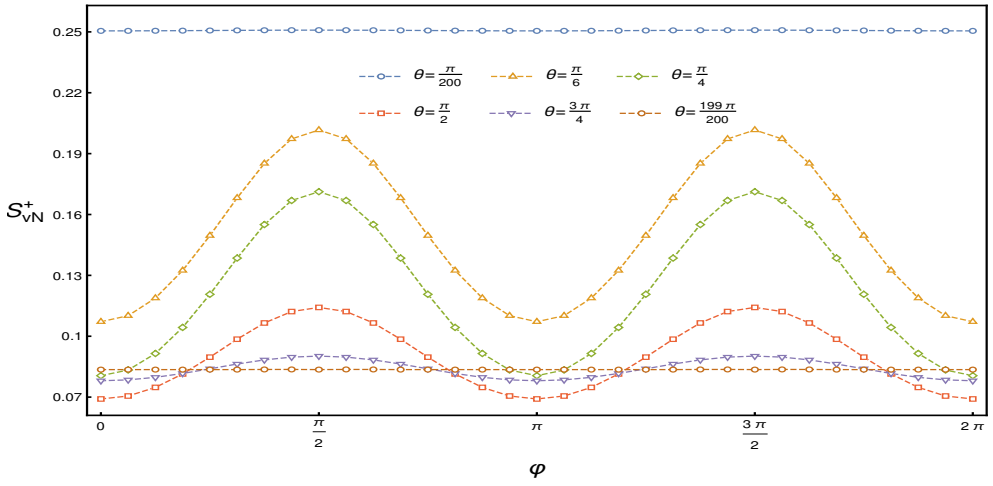
Interestingly the general features are independent of the parameters of the Hamiltonian and one can get universal results for the reduced density matrix and entanglement for generic eigenstates. The procedure used here can be extended for the other similar situations such as local breaking of the parity number symmetry in quantum spin chains due to local magnetic field impurity. It can be also useful to study local quantum quenches in quantum spin chains.



(a) $h = \frac{1}{2}$



(b) $h = 1$



(c) $h = \frac{3}{2}$

Figure 10 – In this figure, the von Neumann entropy is plotted with respect to the angles of BMF, for three values of magnetic field, $h = \frac{1}{2}$, 1, $\frac{3}{2}$ respectively. We have put $b_{1,x} = b_{L,x} = \sin(\theta)\cos(\phi)$, $b_{1,y} = b_{L,y} = \sin(\theta)\sin(\phi)$ and $b_{1,z} = b_{L,z} = \cos(\theta)$. Rest of parameters are: $L = 30$, $l = 2$, $\beta = +1$, $J = -1$ and $\gamma = 1$. To better manifest the change in the entanglement entropy, size of the subsystem is selected to be close to the beginning of the chain. We observe that there is a change in the entanglement at $\varphi = \frac{\pi}{2}, \frac{3\pi}{2}$. As mentioned before, there is (one) more zero mode in the eigenvalues of $\mathbf{M}$ matrix in (7.9) for $h > 1$. However, this is not an exact zero mode and for size $L = 30$, it is small but not zero. Therefore, observation above is intact.

Conclusion

This thesis aimed to lay out a circumstantial explanation of the means and methods of studying XY spin chains and the quadratic fermion models and how these particular families of spin chains are connected to the free fermions models. In part I, the tools provided by quadratic fermion models allow us to calculate the correlation function of either spins or fermions. With the help of these methods, different formulations of density matrix and reduced density matrix were presented. Although these topics are not new and important developments in this line of research was made 50-60 years ago, there is still much to discover and unfold in these models. Moreover, after many decades since the beginning, a comprehensive review of these models has not been presented in the literature. In part II, contains the contributions of my PhD to this field of research, for instance, chapter 6 explains the peculiar behavior of averaging entanglement entropy of subsystems over all eigenstates in these models. The arguments and reasonings of this chapter are mounted in the most general form possible. Chapter 7 provides a good example of utilizing techniques of free fermions to study entanglement contents of an non-integrable spin model. Actually, it provides a computationally simple method to study entanglement in a spin chain with boundary magnetic field, previously thought to be cumbersome and only investigated in special limits.

With any great solvable models, comes limitations. Although interesting fir its own sake, a general quadratic fermion Hamiltonian, in d-dimensions, does not map to a spin model. It is a problem because there has been no consistence definition for a fermionization transformation in $d > 1$ dimensions. While in 1D, the family of XY spin chains are solvable, not all the spin chains obtained by the inverse Jordan-Wigner transformation of a quadratic fermion are practical to study. Another downside to point out is that the general quadratic fermion models lack the possibility of studying interacting fermion models, except a small number of cases. For the future references, one could look at the improvements in emerging quantum simulations and quantum devices using the many-body relations available in free fermions and spin chains. Existing connections among different quantities (correlation, entanglement, full counting statistics) in free fermions can be useful in better quantum

algorithms. Since these models can also be used as a playground to study symmetric field theories and CFT's. it oopens up the possibility to uncover new aspects of theoretical physics.

Referências

1 EINSTEIN, A.; PODOLSKY, B.; ROSEN, N. Can quantum-mechanical description of physical reality be considered complete? *Phys. Rev.*, American Physical Society, v. 47, p. 777–780, May 1935. Disponível em: <https://link.aps.org/doi/10.1103/PhysRev.47.777>. 13

2 BELL, J. S. On the einstein podolsky rosen paradox. *Physics Physique Fizika*, American Physical Society, v. 1, p. 195–200, Nov 1964. Disponível em: <https://link.aps.org/doi/10.1103/PhysicsPhysiqueFizika.1.195>. 13

3 ASPECT, A.; GRANGIER, P.; ROGER, G. Experimental tests of realistic local theories via bell's theorem. *Phys. Rev. Lett.*, American Physical Society, v. 47, p. 460–463, Aug 1981. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevLett.47.460>. 13

4 ASPECT, A.; DALIBARD, J.; ROGER, G. Experimental test of bell's inequalities using time-varying analyzers. *Phys. Rev. Lett.*, American Physical Society, v. 49, p. 1804–1807, Dec 1982. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevLett.49.1804>. 13

5 NIELSEN, M. A.; CHUANG, I. L. *Quantum Computation and Quantum Information: 10th Anniversary Edition*. [S.l.]: Cambridge University Press, 2010. 13

6 BLOCH, I.; DALIBARD, J.; ZWERGER, W. Many-body physics with ultracold gases. *Rev. Mod. Phys.*, American Physical Society, v. 80, p. 885–964, Jul 2008. Disponível em: <https://link.aps.org/doi/10.1103/RevModPhys.80.885>. 13

7 ARUTE, F. et al. Quantum supremacy using a programmable superconducting processor. *Nature*, v. 574, n. 7779, p. 505–510, Oct 2019. ISSN 1476-4687. Disponível em: <https://doi.org/10.1038/s41586-019-1666-5>. 13

8 CALABRESE, P.; CARDY, J. Entanglement entropy and conformal field theory. *Journal of Physics A: Mathematical and Theoretical*, IOP Publishing, v. 42, n. 50, p. 504005, dec 2009. Disponível em: <https://doi.org/10.1088%2F1751-8113%2F42%2F50%2F504005>. 13, 72

9 POLLMANN, F. et al. Entanglement spectrum of a topological phase in one dimension. *Phys. Rev. B*, American Physical Society, v. 81, p. 064439, Feb 2010. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevB.81.064439>. 13

10 LI, H.; HALDANE, F. D. M. Entanglement spectrum as a generalization of entanglement entropy: Identification of topological order in non-abelian fractional quantum hall effect states. *Phys. Rev. Lett.*, American Physical Society, v. 101, p. 010504,

Jul 2008. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevLett.101.010504>. 13

11 QI, X.-L.; KATSURA, H.; LUDWIG, A. W. W. General relationship between the entanglement spectrum and the edge state spectrum of topological quantum states. *Phys. Rev. Lett.*, American Physical Society, v. 108, p. 196402, May 2012. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevLett.108.196402>. 13

12 AMICO, L. et al. Entanglement in many-body systems. *Rev. Mod. Phys.*, American Physical Society, v. 80, p. 517–576, May 2008. Disponível em: <https://link.aps.org/doi/10.1103/RevModPhys.80.517>. 13, 67, 72

13 CHUNG, M.-C.; PESCHEL, I. Density-matrix spectra of solvable fermionic systems. *Phys. Rev. B*, American Physical Society, v. 64, p. 064412, Jul 2001. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevB.64.064412>. 14, 32, 34, 53, 54, 72, 82, 83, 89, 99

14 PESCHEL, I. Calculation of reduced density matrices from correlation functions. *Journal of Physics A: Mathematical and General*, IOP Publishing, v. 36, n. 14, p. L205–L208, mar 2003. Disponível em: <https://doi.org/10.1088%2F0305-4470%2F36%2F14%2F101>. 14, 53, 72, 75, 79, 85, 104

15 PESCHEL, I. On the reduced density matrix for a chain of free electrons. *Journal of Statistical Mechanics: Theory and Experiment*, IOP Publishing, v. 2004, n. 06, p. P06004, jun 2004. Disponível em: <https://doi.org/10.1088/1742-5468/2004/06/p06004>. 14, 82, 83

16 JAFARIZADEH, A.; RAJABPOUR, M. A. Bipartite entanglement entropy of the excited states of free fermions and harmonic oscillators. *Phys. Rev. B*, American Physical Society, v. 100, p. 165135, Oct 2019. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevB.100.165135>. 14, 26, 34, 73, 80, 82

17 JAFARIZADEH, A.; RAJABPOUR, M. A. Entanglement entropy in quantum spin chains with broken parity number symmetry. *SciPost Phys.*, SciPost, v. 12, p. 195, 2022. Disponível em: <https://scipost.org/10.21468/SciPostPhys.12.6.195>. 14, 60

18 Heisenberg, W. Mehrkörperproblem und Resonanz in der Quantenmechanik. *Zeitschrift fur Physik*, v. 38, n. 6-7, p. 411–426, jun 1926. 17

19 DIRAC, P. A. M.; FOWLER, R. H. On the theory of quantum mechanics. *Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character*, v. 112, n. 762, p. 661–677, 1926. Disponível em: <https://royalsocietypublishing.org/doi/abs/10.1098/rspa.1926.0133>. 17

20 Bethe, H. Zur theorie der metalle. *Zeitschrift fur Physik*, v. 71, n. 3-4, p. 205–226, mar. 1931. 17

21 FADDEEV, L. D.; SKLYANIN, E. K.; TAKHTAJAN, L. A. The quantum inverse problem method. 1. *Teor. Mat. Fiz.*, v. 40, p. 194–220, 1979. 17

22 TAKHTAJAN, L. A.; FADDEEV, L. D. The quantum method of the inverse problem and the heisenberg xyz model. *Russ. Math. Surveys*, v. 34, n. 5, p. 11–68, 1979. 17

23 JORDAN, P.; WIGNER, E. P. About the Pauli exclusion principle. *Z. Phys.*, v. 47, p. 631–651, 1928. 17

24 LIEB, E.; SCHULTZ, T.; MATTIS, D. Two soluble models of an antiferromagnetic chain. *Annals of Physics*, v. 16, n. 3, p. 407 – 466, 1961. ISSN 0003-4916. Disponível em: <http://www.sciencedirect.com/science/article/pii/0003491661901154>. 17, 27, 82

25 HENKEL, M. *Conformal Invariance and Critical Phenomena*. Berlin, Heidelberg: Springer Berlin Heidelberg, 1999. 1–42 p. ISBN 978-3-662-03937-3. Disponível em: <https://doi.org/10.1007/978-3-662-03937-3_1>. 17

26 BUNDER, J. E.; MCKENZIE, R. H. Effect of disorder on quantum phase transitions in anisotropic xy spin chains in a transverse field. *Phys. Rev. B*, American Physical Society, v. 60, p. 344–358, Jul 1999. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevB.60.344>. 17

27 FRANCHINI, F. et al. Ellipses of constant entropy in the xy spin chain. *Journal of Physics A: Mathematical and Theoretical*, IOP Publishing, v. 40, n. 29, p. 8467–8478, jul 2007. Disponível em: <https://doi.org/10.1088/1751-8113/40/29/019>. 17

28 FRANCHINI, F.; ITS, A. R.; KOREPIN, V. E. Renyi entropy of the XY spin chain. *Journal of Physics A: Mathematical and Theoretical*, IOP Publishing, v. 41, n. 2, p. 025302, dec 2007. Disponível em: <https://doi.org/10.1088/1751-8113/41/2/025302>. 17

29 EISLER, V. et al. Entanglement evolution after connecting finite to infinite quantum chains. *Journal of Statistical Mechanics: Theory and Experiment*, IOP Publishing, v. 2008, n. 01, p. P01023, jan 2008. Disponível em: <https://doi.org/10.1088/1742-5468/2008/01/p01023>. 17

30 BATLE, J.; CASAS, M. Nonlocality and entanglement in the *XY* model. *Phys. Rev. A*, American Physical Society, v. 82, p. 062101, Dec 2010. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevA.82.062101>. 17

31 WENDENBAUM, P.; PLATINI, T.; KAREVSKI, D. Entanglement replication via quantum repeated interactions. *Phys. Rev. A*, American Physical Society, v. 91, p. 040303, Apr 2015. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevA.91.040303>. 17

32 FRANCHINI, F. et al. Spectrum of the density matrix of a large block of spins of the xy model in one dimension. *Quantum Information Processing*, v. 10, n. 3, p. 325–341, Jun 2011. ISSN 1573-1332. Disponível em: <https://doi.org/10.1007/s11128-010-0197-7>. 17

33 HOEGER, C.; GEHLEN, G. von; RITTENBERG, V. Finite-size scaling for quantum chains with an oscillatory energy gap. *Journal of Physics A: Mathematical and General*, IOP Publishing, v. 18, n. 10, p. 1813–1826, jul 1985. Disponível em: <https://doi.org/10.1088/0305-4470/18/10/033>. 18

34 KURMANN, J.; THOMAS, H.; MüLLER, G. Antiferromagnetic long-range order in the anisotropic quantum spin chain. *Physica A: Statistical Mechanics and its Applications*, v. 112, n. 1, p. 235–255, 1982. ISSN 0378-4371. Disponível em: <https://www.sciencedirect.com/science/article/pii/0378437182902175>. 18, 19

35 SACHDEV, S. *Quantum Phase Transitions*. 2. ed. [S.l.]: Cambridge University Press, 2011. 24, 26

36 BOYANOVSKY, D. Field theory of the two-dimensional ising model: Conformal invariance, order and disorder, and bosonization. *Phys. Rev. B*, American Physical Society, v. 39, p. 6744–6756, Apr 1989. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevB.39.6744>. 24

37 HONGLER, C. *Conformal invariance of Ising model correlations*. Tese (Doutorado) — Univ. Genéve, 06/28 2010. ID: unige:18163. Disponível em: <https://nbn-resolving.org/urn:nbn:ch:unige-181636>. 24

38 TRANSVERSE Ising Chain (Pure System). In: QUANTUM Ising Phases and Transitions in Transverse Ising Models. Berlin, Heidelberg: Springer Berlin Heidelberg, 1996. p. 17–49. ISBN 978-3-540-49865-0. Disponível em: <https://doi.org/10.1007/978-3-540-49865-0_2>. 24

39 FAGOTTI, M. *Entanglement & Correlations in exactly solvable models*. Tese (Doutorado) — The School of Graduate Studies in Basic Sciences "GALILEO GALILEI", Pisa Italy, 2012. Disponível em: <https://scipost.org/theses/18/>. 24, 26, 27, 36, 37, 38, 39, 40, 42, 48, 49, 69

40 KRAMERS, H. A.; WANNIER, G. H. Statistics of the two-dimensional ferromagnet. part i. *Phys. Rev.*, American Physical Society, v. 60, p. 252–262, Aug 1941. Disponível em: <https://link.aps.org/doi/10.1103/PhysRev.60.252>. 24

41 SAVIT, R. Duality in field theory and statistical systems. *Rev. Mod. Phys.*, American Physical Society, v. 52, p. 453–487, Apr 1980. Disponível em: <https://link.aps.org/doi/10.1103/RevModPhys.52.453>. 24

42 FISHER, M. P. A. *Duality in low dimensional quantum field theories*. Dordrecht: Springer Netherlands, 2004. 419–438 p. ISBN 978-1-4020-3463-3. Disponível em: <https://doi.org/10.1007/978-1-4020-3463-3_13>. 24

43 MURAMATSU, A. Lattice gauge theory. 2009. Disponível em: <https://www.itp3.uni-stuttgart.de/downloads/Lattice_gauge_theory_SS_2009/Chapter2.pdf>. 24

44 VENUTI, L. C. et al. Long-distance entanglement and quantum teleportation in xx spin chains. *Phys. Rev. A*, American Physical Society, v. 76, p. 052328, Nov 2007. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevA.76.052328>. 26

45 TACCHINO, F. et al. Quantum computers as universal quantum simulators: State-of-the-art and perspectives. *Advanced Quantum Technologies*, Wiley, v. 3, n. 3, p. 1900052, dec 2019. Disponível em: <https://doi.org/10.1002%2Fqute.201900052>. 26

46 GREINER, M. et al. Quantum phase transition from a superfluid to a mott insulator in a gas of ultracold atoms. *Nature*, v. 415, n. 6867, p. 39–44, Jan 2002. ISSN 1476-4687. Disponível em: <https://doi.org/10.1038/415039a>. 26

47 VIDMAR, L.; RIGOL, M. Entanglement entropy of eigenstates of quantum chaotic hamiltonians. *Phys. Rev. Lett.*, American Physical Society, v. 119, p. 220603, Nov 2017. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevLett.119.220603>. 26, 72

48 NAJAFI, K.; RAJABPOUR, M. A. Full counting statistics of the subsystem energy for free fermions and quantum spin chains. *Phys. Rev. B*, American Physical Society, v. 96, p. 235109, Dec 2017. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevB.96.235109>. 26

49 BAROUCH, E.; MCCOY, B. M.; DRESDEN, M. Statistical mechanics of the XY model. i. *Phys. Rev. A*, American Physical Society, v. 2, p. 1075–1092, Sep 1970. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevA.2.1075>. 27

50 WICK, G. C. The evaluation of the collision matrix. *Phys. Rev.*, American Physical Society, v. 80, p. 268–272, Oct 1950. Disponível em: <https://link.aps.org/doi/10.1103/PhysRev.80.268>. 28, 45, 83

51 KITAEV, A.; LEBEDEV, V.; FEIGEL'MAN, M. Periodic table for topological insulators and superconductors. In: *AIP Conference Proceedings*. AIP, 2009. Disponível em: <https://doi.org/10.1063%2F1.3149495>. 28

52 HEMMEN, J. L. van. A note on the diagonalization of quadratic boson and fermion hamiltonians. *Zeitschrift für Physik B Condensed Matter*, v. 38, n. 3, p. 271–277, Sep 1980. ISSN 1431-584X. Disponível em: <https://doi.org/10.1007/BF01315667>. 31

53 COZZINI, M.; GIORDA, P.; ZANARDI, P. Quantum phase transitions and quantum fidelity in free fermion graphs. *Phys. Rev. B*, American Physical Society, v. 75, p. 014439, Jan 2007. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevB.75.014439>. 33, 90

54 PASQUALE, A. D.; FACCHI, P. *xy* model on the circle: Diagonalization, spectrum, and forerunners of the quantum phase transition. *Phys. Rev. A*, American Physical Society, v. 80, p. 032102, Sep 2009. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevA.80.032102>. 37

55 NOSCHESE, S.; PASQUINI, L.; REICHEL, L. Tridiagonal toeplitz matrices: properties and novel applications. *Numerical Linear Algebra with Applications*, v. 20, n. 2, p. 302–326, 2013. Disponível em: <https://onlinelibrary.wiley.com/doi/abs/10.1002/nla.1811>. 41

56 YUEH, W.-C. Eigenvalues of several tridiagonal matrices. *Applied Mathematics E-Notes [electronic only]*, Department of Mathematics, Tsing Hua University, v. 5, p. 66–74, 2005. Disponível em: <http://eudml.org/doc/51497>. 41

57 SETHNA, J. P. *Statistical Mechanics: Entropy, Order Parameters, and Complexity: Second Edition*. 2. ed. Oxford: Oxford University Press, 2021. 496 p. (Oxford Master Series in Physics). ISBN 9780198865247. Disponível em: <https://doi.org/10.1093/oso/9780198865247.001.0001>. 45

58 CARACCIOLO, S.; SOKAL, A. D.; SPORTIELLO, A. Algebraic/combinatorial proofs of cayley-type identities for derivatives of determinants and pfaffians. *Advances in Applied Mathematics*, v. 50, n. 4, p. 474 – 594, 2013. ISSN 0196-8858. Disponível em: <http://www.sciencedirect.com/science/article/pii/S0196885812001315>. 54, 138, 169

59 BENNETT, C. H. et al. Teleporting an unknown quantum state via dual classical and einstein-podolsky-rosen channels. *Phys. Rev. Lett.*, American Physical Society, v. 70, p. 1895–1899, Mar 1993. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevLett.70.1895>. 67

60 EKERT, A. K. Quantum cryptography based on bell's theorem. *Phys. Rev. Lett.*, American Physical Society, v. 67, p. 661–663, Aug 1991. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevLett.67.661>. 67

61 PLENIO, M. B.; VIRMANI, S. An introduction to entanglement measures. *Quantum Inf. Comput.*, v. 7, n. 1, p. 1–51, 2007. Disponível em: <https://doi.org/10.26421/QIC7.1-2-1>. 67

62 HORODECKI, R. et al. Quantum entanglement. *Rev. Mod. Phys.*, American Physical Society, v. 81, p. 865–942, Jun 2009. Disponível em: <https://link.aps.org/doi/10.1103/RevModPhys.81.865>. 67

63 EISERT, J. Entanglement in quantum information theory. arXiv, 2006. Disponível em: <https://arxiv.org/abs/quant-ph/0610253>. 67

64 BENGTSSON, I.; ZYCZKOWSKI, K. *Geometry of Quantum States: An Introduction to Quantum Entanglement*. [S.l.]: Cambridge University Press, 2006. 67

65 VIDAL, G. et al. Entanglement in quantum critical phenomena. *Phys. Rev. Lett.*, American Physical Society, v. 90, p. 227902, Jun 2003. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevLett.90.227902>. 67, 68, 72, 82, 83, 108

66 LATORRE, J. I.; RICO, E.; VIDAL, G. Ground state entanglement in quantum spin chains. *Quantum Info. Comput.*, Rinton Press, Incorporated, Paramus, NJ, v. 4, n. 1, p. 48–92, jan 2004. ISSN 1533-7146. 67, 83

67 JIN, B.-Q.; KOREPIN, V. E. Quantum spin chain, toeplitz determinants and the fisher—hartwig conjecture. *Journal of Statistical Physics*, v. 116, n. 1, p. 79–95, Aug 2004. Disponível em: <https://doi.org/10.1023/B:JOSS.0000037230.37166.42>. 68, 72, 82, 83, 108

68 KEATING, J. P.; MEZZADRI, F. Random matrix theory and entanglement in quantum spin chains. *Communications in Mathematical Physics*, v. 252, n. 1, p. 543–579, Dec 2004. ISSN 1432-0916. Disponível em: <https://doi.org/10.1007/s00220-004-1188-2>. 68, 82, 108

69 PESCHEL, I.; EISLER, V. Reduced density matrices and entanglement entropy in free lattice models. *Journal of Physics A: Mathematical and Theoretical*, IOP Publishing, v. 42, n. 50, p. 504003, dec 2009. Disponível em: <https://doi.org/10.1088%2F1751-8113%2F42%2F50%2F504003>. 68, 72, 82, 108, 160

70 WEHRL, A. General properties of entropy. *Rev. Mod. Phys.*, American Physical Society, v. 50, p. 221–260, Apr 1978. Disponível em: <https://link.aps.org/doi/10.1103/RevModPhys.50.221>. 69

71 CALABRESE, P.; LEFEVRE, A. Entanglement spectrum in one-dimensional systems. *Phys. Rev. A*, American Physical Society, v. 78, p. 032329, Sep 2008. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevA.78.032329>. 69

72 SORKIN, R. D. 1983 paper on entanglement entropy: "on the entropy of the vacuum outside a horizon". *Tenth International Conference on General Relativity and Gravitation*, arXiv, II, p. 734–736, July 1983. Disponível em: <https://arxiv.org/abs/1402.3589>. 72

73 BOMBELLI, L. et al. Quantum source of entropy for black holes. *Phys. Rev. D*, American Physical Society, v. 34, p. 373–383, Jul 1986. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevD.34.373>. 72

74 SREDNICKI, M. Entropy and area. *Phys. Rev. Lett.*, American Physical Society, v. 71, p. 666–669, Aug 1993. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevLett.71.666>. 72

75 HOLZHEY, C.; LARSEN, F.; WILCZEK, F. Geometric and renormalized entropy in conformal field theory. *Nuclear Physics B*, v. 424, n. 3, p. 443 – 467, 1994. ISSN 0550-3213. Disponível em: <http://www.sciencedirect.com/science/article/pii/0550321394904022>. 72, 73

76 GIOEV, D.; KLICH, I. Entanglement entropy of fermions in any dimension and the widom conjecture. *Phys. Rev. Lett.*, American Physical Society, v. 96, p. 100503, Mar 2006. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevLett.96.100503>. 72

77 AUDENAERT, K. et al. Entanglement properties of the harmonic chain. *Phys. Rev. A*, American Physical Society, v. 66, p. 042327, Oct 2002. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevA.66.042327>. 72

78 OSTERLOH, A. et al. Scaling of entanglement close to a quantum phase transition. *Nature*, Nature Publishing Group, v. 416, n. 6881, p. 608, 2002. Disponível em: <https://doi.org/10.1038/416608a>. 72

79 OSBORNE, T. J.; NIELSEN, M. A. Entanglement in a simple quantum phase transition. *Phys. Rev. A*, American Physical Society, v. 66, p. 032110, Sep 2002. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevA.66.032110>. 72

80 HASTINGS, M. B. An area law for one-dimensional quantum systems. *Journal of Statistical Mechanics: Theory and Experiment*, IOP Publishing, v. 2007, n. 08, p. P08024–P08024, aug 2007. Disponível em: <https://doi.org/10.1088%2F1742-5468%2F2007%2F08%2Fp08024>. 72, 73

81 CALABRESE, P.; CARDY, J. Entanglement entropy and quantum field theory. *Journal of Statistical Mechanics: Theory and Experiment*, IOP Publishing, v. 2004, n. 06, p. P06002, 2004. Disponível em: <https://doi.org/10.1088%2F1742-5468%2F2004%2F06%2Fp06002>. 72, 73

82 KITAEV, A.; PRESKILL, J. Topological entanglement entropy. *Phys. Rev. Lett.*, American Physical Society, v. 96, p. 110404, Mar 2006. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevLett.96.110404>. 72

83 LEVIN, M.; WEN, X.-G. Detecting topological order in a ground state wave function. *Phys. Rev. Lett.*, American Physical Society, v. 96, p. 110405, Mar 2006. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevLett.96.110405>. 72

84 AFFLECK, I.; LAFLORENCIE, N.; SØRENSEN, E. S. Entanglement entropy in quantum impurity systems and systems with boundaries. *Journal of Physics A: Mathematical and Theoretical*, IOP Publishing, v. 42, n. 50, p. 504009, dec 2009. Disponível em: <https://doi.org/10.1088%2F1751-8113%2F42%2F50%2F504009>. 72, 82

85 REFAEL, G.; MOORE, J. E. Criticality and entanglement in random quantum systems. *Journal of Physics A: Mathematical and Theoretical*, IOP Publishing, v. 42, n. 50, p. 504010, dec 2009. Disponível em: <https://doi.org/10.1088%2F1751-8113%2F42%2F50%2F504010>. 72

86 EISERT, J.; CRAMER, M.; PLENIO, M. B. Colloquium: Area laws for the entanglement entropy. *Rev. Mod. Phys.*, American Physical Society, v. 82, p. 277–306, Feb 2010. Disponível em: <https://link.aps.org/doi/10.1103/RevModPhys.82.277>. 72

87 MODI, K. et al. The classical-quantum boundary for correlations: Discord and related measures. *Rev. Mod. Phys.*, American Physical Society, v. 84, p. 1655–1707, Nov 2012. Disponível em: <https://link.aps.org/doi/10.1103/RevModPhys.84.1655>. 72

88 LAFLORENCIE, N. Quantum entanglement in condensed matter systems. *Physics Reports*, Elsevier, v. 646, p. 1–59, 2016. ISSN 0370-1573. Disponível em: <http://www.sciencedirect.com/science/article/pii/S0370157316301582>. 72

89 CHIARA, G. D.; SANPERA, A. Genuine quantum correlations in quantum many-body systems: a review of recent progress. *Reports on Progress in Physics*, IOP Publishing, v. 81, n. 7, p. 074002, jun 2018. Disponível em: <https://doi.org/10.1088%2F1361-6633%2Faabf61>. 72

90 CASTRO-ALVAREDO, O. A.; DOYON, B. Bi-partite entanglement entropy in massive (1+1)-dimensional quantum field theories. *Journal of Physics A: Mathematical and Theoretical*, IOP Publishing, v. 42, n. 50, p. 504006, dec 2009. Disponível em: <https://doi.org/10.1088%2F1751-8113%2F42%2F50%2F504006>. 72

91 CASINI, H.; HUERTA, M. Entanglement entropy in free quantum field theory. *Journal of Physics A: Mathematical and Theoretical*, IOP Publishing, v. 42, n. 50, p. 504007, dec 2009. Disponível em: <https://doi.org/10.1088%2F1751-8113%2F42%2F50%2F504007>. 72, 160

92 ALBA, V.; FAGOTTI, M.; CALABRESE, P. Entanglement entropy of excited states. *Journal of Statistical Mechanics: Theory and Experiment*, IOP Publishing, v. 2009, n. 10, p. P10020, oct 2009. 72, 73, 75, 82

93 ARES, F. et al. Excited state entanglement in homogeneous fermionic chains. *Journal of Physics A: Mathematical and Theoretical*, IOP Publishing, v. 47, n. 24, p. 245301, jun 2014. Disponível em: <https://doi.org/10.1088%2F1751-8113%2F47%2F24%2F245301>. 72, 73, 76, 82

94 ALCARAZ, F. C.; BERGANZA, M. I. n.; SIERRA, G. Entanglement of low-energy excitations in conformal field theory. *Phys. Rev. Lett.*, American Physical Society, v. 106, p. 201601, May 2011. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevLett.106.201601>. 72, 82

95 BERGANZA, M. I.; ALCARAZ, F. C.; SIERRA, G. Entanglement of excited states in critical spin chains. *Journal of Statistical Mechanics: Theory and Experiment*, IOP Publishing, v. 2012, n. 01, p. P01016, jan 2012. Disponível em: <https://doi.org/10.1088%2F1742-5468%2F2012%2F01%2Fp01016>. 72, 82

96 MöLTER, J. et al. Bound states and entanglement in the excited states of quantum spin chains. *Journal of Statistical Mechanics: Theory and Experiment*, IOP Publishing, v. 2014, n. 10, p. P10029, oct 2014. Disponível em: <https://doi.org/10.1088%2F1742-5468%2F2014%2F10%2Fp10029>. 72

97 STORMS, M.; SINGH, R. R. P. Entanglement in ground and excited states of gapped free-fermion systems and their relationship with fermi surface and thermodynamic equilibrium properties. *Phys. Rev. E*, American Physical Society, v. 89, p. 012125, Jan 2014. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevE.89.012125>. 72

98 BEUGELING, W.; ANDREANOV, A.; HAQUE, M. Global characteristics of all eigenstates of local many-body hamiltonians: participation ratio and entanglement entropy. *Journal of Statistical Mechanics: Theory and Experiment*, IOP Publishing, v. 2015, n. 2, p. P02002, feb 2015. Disponível em: <https://doi.org/10.1088%2F1742-5468%2F2015%2F02%2Fp02002>. 72

99 LAI, H.-H.; YANG, K. Entanglement entropy scaling laws and eigenstate typicality in free fermion systems. *Phys. Rev. B*, American Physical Society, v. 91, p. 081110, Feb 2015. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevB.91.081110>. 72

100 ALBA, V. Eigenstate thermalization hypothesis and integrability in quantum spin chains. *Phys. Rev. B*, American Physical Society, v. 91, p. 155123, Apr 2015. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevB.91.155123>. 72

101 NANDY, S. et al. Eigenstate gibbs ensemble in integrable quantum systems. *Phys. Rev. B*, American Physical Society, v. 94, p. 245131, Dec 2016. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevB.94.245131>. 72

102 VIDMAR, L. et al. Entanglement entropy of eigenstates of quadratic fermionic hamiltonians. *Phys. Rev. Lett.*, American Physical Society, v. 119, p. 020601, Jul 2017. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevLett.119.020601>. 72, 73, 78, 79, 80, 82, 161

103 RIDDELL, J.; MÜLLER, M. P. Generalized eigenstate typicality in translation-invariant quasifree fermionic models. *Phys. Rev. B*, American Physical Society, v. 97, p. 035129, Jan 2018. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevB.97.035129>. 72

104 ZHANG, Y.; VIDMAR, L.; RIGOL, M. Information measures for a local quantum phase transition: Lattice fermions in a one-dimensional harmonic trap. *Phys. Rev. A*, American Physical Society, v. 97, p. 023605, Feb 2018. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevA.97.023605>. 72

105 LIU, C.; CHEN, X.; BALENTS, L. Quantum entanglement of the sachdev-ye-kitaev models. *Phys. Rev. B*, American Physical Society, v. 97, p. 245126, Jun 2018. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevB.97.245126>. 72

106 VIDMAR, L. et al. Volume law and quantum criticality in the entanglement entropy of excited eigenstates of the quantum ising model. *Phys. Rev. Lett.*, American Physical Society, v. 121, p. 220602, Nov 2018. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevLett.121.220602>. 72, 73, 78, 79, 80

107 HACKL, L. et al. Average eigenstate entanglement entropy of the xy chain in a transverse field and its universality for translationally invariant quadratic fermionic models. *Phys. Rev. B*, American Physical Society, v. 99, p. 075123, Feb 2019. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevB.99.075123>. 72, 73, 82

108 MIAO, Q.; BARTHEL, T. Eigenstate entanglement: Crossover from the ground state to volume laws. *arXiv preprint arXiv:1905.07760*, 2019. Disponível em: <https://arxiv.org/abs/1905.07760>. 72

109 Lu, T.-C.; Grover, T. Renyi entropy of chaotic eigenstates. *Physical Review E*, v. 99, n. 22, p. 032111, March 2019. 72

110 MURTHY, C.; SREDNICKI, M. The structure of chaotic eigenstates and their entanglement entropy. *arXiv preprint arXiv:1906.04295*, 2019. Disponível em: <https://arxiv.org/abs/1906.04295>. 72

111 TADDIA, L. et al. Entanglement entropies in conformal systems with boundaries. *Phys. Rev. B*, American Physical Society, v. 88, p. 075112, Aug 2013. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevB.88.075112>. 72, 82

112 HERWERTH, B. et al. Excited states in spin chains from conformal blocks. *Phys. Rev. B*, American Physical Society, v. 91, p. 235121, Jun 2015. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevB.91.235121>. 72

113 PÁLMAI, T. Excited state entanglement in one-dimensional quantum critical systems: Extensivity and the role of microscopic details. *Phys. Rev. B*, American Physical Society, v. 90, p. 161404, Oct 2014. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevB.90.161404>. 72

114 TADDIA, L.; ORTOLANI, F.; PÁLMAI, T. Renyi entanglement entropies of descendant states in critical systems with boundaries: conformal field theory and spin chains. *Journal of Statistical Mechanics: Theory and Experiment*, IOP Publishing, v. 2016, n. 9, p. 093104, sep 2016. Disponível em: <https://doi.org/10.1088%2F1742-5468%2F2016%2F09%2F093104>. 72

115 RUGGIERO, P.; CALABRESE, P. Relative entanglement entropies in 1 + 1-dimensional conformal field theories. *Journal of High Energy Physics*, v. 2017, n. 2, p. 39, Feb 2017. ISSN 1029-8479. Disponível em: <https://doi.org/10.1007/JHEP02(2017)039>. 72

116 ZHANG, J.; RUGGIERO, P.; CALABRESE, P. Subsystem trace distance in quantum field theory. *Phys. Rev. Lett.*, American Physical Society, v. 122, p. 141602, Apr 2019. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevLett.122.141602>. 72

117 ZHANG, J.; RUGGIERO, P.; CALABRESE, P. Subsystem trace distance in low-lying states of conformal field theories. *arXiv preprint arXiv:1907.04332*, 2019. Disponível em: <https://arxiv.org/abs/1907.04332>. 72

118 CASTRO-ALVAREDO, O. A. et al. Entanglement content of quasiparticle excitations. *Phys. Rev. Lett.*, American Physical Society, v. 121, p. 170602, Oct 2018. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevLett.121.170602>. 72

119 CASTRO-ALVAREDO, O. A. et al. Entanglement content of quantum particle excitations. part i. free field theory. *Journal of High Energy Physics*, v. 2018, n. 10, p. 39, Oct 2018. ISSN 1029-8479. Disponível em: <https://doi.org/10.1007/JHEP10(2018)039>. 72

120 CARRASCO, J. A. et al. A duality principle for the multi-block entanglement entropy of free fermion systems. *Scientific Reports*, v. 7, n. 1, p. 11206, 2017. ISSN 2045-2322. Disponível em: <https://doi.org/10.1038/s41598-017-09550-1>. 73, 79

121 VERRESEN, R.; JONES, N. G.; POLLMANN, F. Topology and edge modes in quantum critical chains. *Phys. Rev. Lett.*, American Physical Society, v. 120, p. 057001, Jan 2018. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevLett.120.057001>. 74, 75

122 ELBEN, A. et al. Rényi entropies from random quenches in atomic hubbard and spin models. *Phys. Rev. Lett.*, American Physical Society, v. 120, p. 050406, Feb 2018. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevLett.120.050406>. 80

123 BRYDGES, T. et al. Probing rényi entanglement entropy via randomized measurements. *Science*, American Association for the Advancement of Science, v. 364, n. 6437, p. 260–263, 2019. ISSN 0036-8075. Disponível em: <https://science.sciencemag.org/content/364/6437/260>. 80

124 IGLóI, F.; PESCHEL, I. On reduced density matrices for disjoint subsystems. *EPL*, American Physical Society, v. 89, p. 40001, Aug 2010. Disponível em: <https://iopscience.iop.org/article/10.1209/0295-5075/89/40001>. 80, 82, 106, 110

125 FRANCHINI, F.; ABANOV, A. G. Asymptotics of toeplitz determinants and the emptiness formation probability for the XY spin chain. *Journal of Physics A: Mathematical and General*, IOP Publishing, v. 38, n. 23, p. 5069–5095, may 2005. Disponível em: <https://doi.org/10.1088/0305-4470/38/23/002>. 82

126 NAJAFI, K.; RAJABPOUR, M. A. Formation probabilities and shannon information and their time evolution after quantum quench in the transverse-field xy chain. *Phys. Rev. B*, American Physical Society, v. 93, p. 125139, Mar 2016. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevB.93.125139>. 82

127 NAJAFI, M. N.; RAJABPOUR, M. A. Formation probabilities and statistics of observables as defect problems in free fermions and quantum spin chains. *Phys. Rev. B*, American Physical Society, v. 101, p. 165415, Apr 2020. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevB.101.165415>. 82

128 Zhang, J.; Rajabpour, M. A. Universal Rényi Entropy of Quasiparticle Excitations. *arXiv e-prints*, p. arXiv:2010.13973, out. 2020. 82

129 Zhang, J.; Rajabpour, M. A. Universal Rényi entropy in quasiparticle excited states of quantum chains. *arXiv e-prints*, p. arXiv:2010.16348, out. 2020. 82

130 LAFLORENCIE, N. et al. Boundary effects in the critical scaling of entanglement entropy in 1d systems. *Phys. Rev. Lett.*, American Physical Society, v. 96, p. 100603, Mar 2006. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevLett.96.100603>. 82

131 ZHOU, H.-Q. et al. Entanglement and boundary critical phenomena. *Phys. Rev. A*, American Physical Society, v. 74, p. 050305, Nov 2006. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevA.74.050305>. 82

132 LEGEZA, O. et al. Entropic analysis of quantum phase transitions from uniform to spatially inhomogeneous phases. *Phys. Rev. Lett.*, American Physical Society, v. 99, p. 087203, Aug 2007. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevLett.99.087203>. 82

133 SZIRMAI, E.; LEGEZA, O.; SÓLYOM, J. Spatially nonuniform phases in the one-dimensional SU(n) hubbard model for commensurate fillings. *Phys. Rev. B*, American Physical Society, v. 77, p. 045106, Jan 2008. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevB.77.045106>. 82

134 CASTRO-ALVAREDO, O. A.; DOYON, B. Bi-partite entanglement entropy in massive qft with a boundary: the ising model. *Journal of Statistical Physics*, v. 134, Jan 2009. Disponível em: <https://doi.org/10.1007/s10955-008-9664-2>. 82

135 FAGOTTI, M.; CALABRESE, P. Universal parity effects in the entanglement entropy of xx chains with open boundary conditions. *Journal of Statistical Mechanics: Theory and Experiment*, IOP Publishing, v. 2011, n. 01, p. P01017, jan 2011. Disponível em: <https://doi.org/10.1088/1742-5468/2011/01/p01017>. 82, 107

136 BRAVYI, S. B.; KITAEV, A. Y. Fermionic quantum computation. *Annals of Physics*, v. 298, n. 1, p. 210–226, 2002. ISSN 0003-4916. Disponível em: <https://www.sciencedirect.com/science/article/pii/S0003491602962548>. 82

137 NULS, M.-C. B.; CIRAC, J. I.; WOLF, M. M. Entanglement in fermionic systems. *Phys. Rev. A*, American Physical Society, v. 76, p. 022311, Aug 2007. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevA.76.022311>. 82

138 MORIYA, H. On separable states for composite systems of distinguishable fermions. *Journal of Physics A: Mathematical and General*, IOP Publishing, v. 39, n. 14, p. 3753, 2006. 82

139 VEGA, H. J. de; RUIZ, A. G. Boundary k-matrices for the six vertex and the n(2n-1)an-1vertex models. *Journal of Physics A: Mathematical and General*, IOP Publishing, v. 26, n. 12, p. L519–L524, jun 1993. Disponível em: <https://doi.org/10.1088/0305-4470/26/12/007>. 82

140 NEPOMECHIE, R. I. Solving the open xxz spin chain with nondiagonal boundary terms at roots of unity. *Nuclear Physics B*, v. 622, n. 3, p. 615–632, 2002. ISSN 0550-3213. Disponível em: <https://www.sciencedirect.com/science/article/pii/S0550321301005855>. 82

141 NEPOMECHIE, R. I. Bethe ansatz solution of the open XXZ chain with nondiagonal boundary terms. *Journal of Physics A: Mathematical and General*, IOP Publishing, v. 37, n. 2, p. 433–440, dec 2003. Disponível em: <https://doi.org/10.1088/0305-4470/37/2/012>. 82

142 CAO, J. et al. Exact solution of xxz spin chain with unparallel boundary fields. *Nuclear Physics B*, v. 663, n. 3, p. 487–519, 2003. ISSN 0550-3213. Disponível em: <https://www.sciencedirect.com/science/article/pii/S0550321303003729>. 82

143 CAO, J. et al. Off-diagonal bethe ansatz solution of the xxx spin chain with arbitrary boundary conditions. *Nuclear Physics B*, v. 875, n. 1, p. 152–165, 2013. ISSN 0550-3213.

Disponível em: <https://www.sciencedirect.com/science/article/pii/S0550321313003507>. 82

144 CAO, J. et al. Off-diagonal bethe ansatz solutions of the anisotropic spin-12 chains with arbitrary boundary fields. *Nuclear Physics B*, v. 877, n. 1, p. 152–175, 2013. ISSN 0550-3213. Disponível em: <https://www.sciencedirect.com/science/article/pii/S0550321313005014>. 82

145 NICCOLI, G. Antiperiodic spin-1/2 xxz quantum chains by separation of variables: Complete spectrum and form factors. *Nuclear Physics B*, v. 870, n. 2, p. 397–420, 2013. ISSN 0550-3213. Disponível em: <https://www.sciencedirect.com/science/article/pii/S0550321313000540>. 82

146 BELLIARD, S.; CRAMPÉ, N. et al. Heisenberg xxx model with general boundaries: eigenvectors from algebraic bethe ansatz. *SIGMA. Symmetry, Integrability and Geometry: Methods and Applications*, SIGMA. Symmetry, Integrability and Geometry: Methods and Applications, v. 9, p. 072, 2013. 82

147 NEPOMECHIE, R. I.; WANG, C. Boundary energy of the open XXX chain with a non-diagonal boundary term. *Journal of Physics A: Mathematical and Theoretical*, IOP Publishing, v. 47, n. 3, p. 032001, dec 2013. Disponível em: <https://doi.org/10.1088/1751-8113/47/3/032001>. 82

148 FALDELLA, S.; KITANINE, N.; NICCOLI, G. The complete spectrum and scalar products for the open spin-1/2 XXZ quantum chains with non-diagonal boundary terms. *Journal of Statistical Mechanics: Theory and Experiment*, IOP Publishing, v. 2014, n. 1, p. P01011, jan 2014. Disponível em: <https://doi.org/10.1088/1742-5468/2014/01/p01011>. 82

149 KITANINE, N.; MAILLET, J. M.; NICCOLI, G. Open spin chains with generic integrable boundaries: Baxter equation and bethe ansatz completeness from separation of variables. *Journal of Statistical Mechanics: Theory and Experiment*, IOP Publishing, v. 2014, n. 5, p. P05015, may 2014. Disponível em: <https://doi.org/10.1088/1742-5468/2014/05/p05015>. 82

150 LI, Y.-Y. et al. Thermodynamic limit and surface energy of the xxz spin chain with arbitrary boundary fields. *Nuclear Physics B*, v. 884, p. 17–27, 2014. ISSN 0550-3213. Disponível em: <https://www.sciencedirect.com/science/article/pii/S0550321314001199>. 82

151 POZSGAY, B.; RÁKOS, O. Exact boundary free energy of the open XXZ chain with arbitrary boundary conditions. *Journal of Statistical Mechanics: Theory and Experiment*, IOP Publishing, v. 2018, n. 11, p. 113102, nov 2018. Disponível em: <https://doi.org/10.1088/1742-5468/aae5a5>. 82

152 COLPA, J. H. P. Diagonalisation of the quadratic fermion hamiltonian with a linear part. *Journal of Physics A: Mathematical and General*, IOP Publishing, v. 12, n. 4, p. 469–488, apr 1979. Disponível em: <https://doi.org/10.1088%2F0305-4470%2F12%2F4%2F008>. 82, 83, 85, 176

153 BARIEV, R.; PESCHEL, I. Non-universal critical behaviour in a two-dimensional ising model with a field. *Physics Letters A*, v. 153, n. 4, p. 166–168, 1991. ISSN 0375-9601.

Disponível em: <https://www.sciencedirect.com/science/article/pii/0375960191907868>. 82, 85

154 BILSTEIN, U.; WEHEFRITZ, B. The -model with boundaries: Part i. diagonalization of the finite chain. *Journal of Physics A: Mathematical and General*, IOP Publishing, v. 32, n. 2, p. 191–233, jan 1999. Disponível em: <https://doi.org/10.1088/0305-4470/32/2/001>. 82, 83, 85, 86

155 CAMPOSTRINI, M.; PELISSETTO, A.; VICARI, E. Quantum ising chains with boundary fields. *Journal of Statistical Mechanics: Theory and Experiment*, IOP Publishing, v. 2015, n. 11, p. P11015, nov 2015. Disponível em: <https://doi.org/10.1088/1742-5468/2015/11/p11015>. 82, 85

156 XAVIER, J. C.; RAJABPOUR, M. A. Entanglement and boundary entropy in quantum spin chains with arbitrary direction of the boundary magnetic fields. *Phys. Rev. B*, American Physical Society, v. 101, p. 235127, Jun 2020. Disponível em: <https://link.aps.org/doi/10.1103/PhysRevB.101.235127>. 82, 83, 85, 86, 91, 101, 102, 110, 112, 114

157 BALIAN, R.; BREZIN, E. Nonunitary bogoliubov transformations and extension of wick's theorem. *Il Nuovo Cimento B (1965-1970)*, v. 64, n. 1, p. 37–55, Nov 1969. ISSN 1826-9877. Disponível em: <https://doi.org/10.1007/BF02710281>. 173

Apêndices

— A —

Grassmann variables and integrals

Grassmann algebra and integration

Grassmann numbers are defined by their anti-commutation. That is given two Grassmann numbers ξ_i and ξ_j, we have

$$\{\xi_n, \xi_m\} = 0 \tag{A.1}$$

In particular, this means that given an anti-commuting number ξ_l, it satisfies $\xi_l^2 = 0$, known as nilpotent with degree 2. The complex conjugates of Grassmann variables, $\bar{\xi}$, are defined similarly:

$$\{\xi_n, \xi_m\} = \{\xi_n, \bar{\xi}_m\} = \{\bar{\xi}_n, \bar{\xi}_m\} = 0. \tag{A.2}$$

It is of interest to point out that the most general function of a Grassmann variable ξ can be written as

$$\mathrm{f}(\xi) = a + b\xi, \tag{A.3}$$

where a and b are normal constants, that is it is at most linear in ξ due to nilpotent condition. I would like to present the integral over Grassmann variable as defined by Berezin:

$$\int d\xi_n = \int d\bar{\xi}_n = 0 \qquad \int d\xi_n \xi_m = \int d\bar{\xi}_n \bar{\xi}_m = \delta_{nm}. \tag{A.4}$$

In the following, I listed some Gaussian integrals regarding the Grassmann variables. For more details of see [58]. Consider the following notation: $\mathbf{A}$ is an antisymmetric matrix with size $2n \times 2n$, $\mathbf{C}$ is an arbitrary matrix with size $r \times 2n$ and pf[$\mathbf{M}$] is called the Pfaffian of the matrix $\mathbf{M}$.

$$\int \prod_l \mathrm{d}\xi_l \mathrm{d}\bar{\xi}_l \, e^{\bar{\boldsymbol{\xi}} \mathbf{A} \boldsymbol{\xi}} = \det(\mathbf{A}) \tag{A.5}$$

$$\int \prod_l \mathrm{d}\xi_l \mathrm{d}\bar{\xi}_l \, e^{\bar{\boldsymbol{\xi}} \mathbf{A} \boldsymbol{\xi} + \bar{\boldsymbol{\lambda}} \boldsymbol{\xi} + \bar{\boldsymbol{\xi}} \boldsymbol{\lambda}} = \det(\mathbf{A}) e^{-\bar{\boldsymbol{\lambda}} \mathbf{A}^{-1} \boldsymbol{\lambda}} \tag{A.6}$$

$$\int \prod_l \mathrm{d}\xi_l \, e^{\frac{1}{2} \boldsymbol{\xi}^T \mathbf{A} \boldsymbol{\xi} + \boldsymbol{\lambda}^T \boldsymbol{\xi}} = \mathrm{pf}[\mathbf{A}] e^{\frac{1}{2} \boldsymbol{\lambda}^T \mathbf{A}^{-1} \boldsymbol{\lambda}} \tag{A.7}$$

$$\int \prod_l \mathrm{d}\xi_l \, (\prod_{i \in J} \xi_i) \, e^{\frac{1}{2} \boldsymbol{\xi}^T \mathbf{A} \boldsymbol{\xi}} = \begin{cases} 0 & J \text{ odd} \\ \mathrm{pf}[\mathbf{A}] \, \mathrm{pf}[(\mathbf{A}^{-T})_{JJ}] & J \text{ even} \end{cases} \tag{A.8}$$

$$\int \prod_l \mathrm{d}\xi_l \, (\mathbf{C}\boldsymbol{\xi})_1 \cdots (\mathbf{C}\boldsymbol{\xi})_r \, e^{\frac{1}{2} \boldsymbol{\xi}^T \mathbf{A} \boldsymbol{\xi}} = \begin{cases} 0 & r \text{ odd} \\ \mathrm{pf}[\mathbf{A}] \, \mathrm{pf}[\mathbf{C}\mathbf{A}^{-T}\mathbf{C}^T] & r \text{ even} \end{cases} \tag{A.9}$$

Fermionic coherent states

In this section, I introduce the fermionic coherent state which is a very useful representation to simplify some calculations. It is defined as

$$|\boldsymbol{\xi}\rangle = |\xi_1, \xi_2, ..., \xi_N\rangle = e^{-\sum_{k=1}^{N} \xi_k c_k^\dagger}|0\rangle, \tag{A.10}$$

where ξ_k's are Grassmann variables. It satisfies the following simple property

$$c_i\,|\boldsymbol{\xi}\rangle = \xi_i|\boldsymbol{\xi}\rangle, \qquad \langle\boldsymbol{\xi}|c_i^\dagger = \langle\boldsymbol{\xi}|\bar{\xi}_i. \tag{A.11}$$

The overlap can be calculated easily as

$$\langle\boldsymbol{\xi}|\boldsymbol{\xi}'\rangle = e^{\bar{\boldsymbol{\xi}}.\boldsymbol{\xi}'}. \tag{A.12}$$

For coherent states the closure relation may be written as

$$\int \prod_i d\bar{\xi}_i d\xi_i e^{-\bar{\boldsymbol{\xi}}.\boldsymbol{\xi}}|\boldsymbol{\xi}\rangle\langle\boldsymbol{\xi}| = 1. \tag{A.13}$$

Using the above equation one can simply expand any state in the coherent basis as follows

$$|\psi\rangle = \int \prod_i d\bar{\xi}_i d\xi_i e^{-\bar{\boldsymbol{\xi}}.\boldsymbol{\xi}}\psi(\bar{\boldsymbol{\xi}})|\boldsymbol{\xi}\rangle, \tag{A.14}$$

where $\psi(\bar{\boldsymbol{\xi}}) = \langle\boldsymbol{\xi}|\psi\rangle$. The other important formula is the trace of an arbitrary operator in the coherent basis. It has the following form

$$\mathrm{tr}\mathcal{O} = \int \prod_i \mathrm{d}\bar{\xi}_i \mathrm{d}\xi_i e^{-\bar{\boldsymbol{\xi}}.\boldsymbol{\xi}}\,\langle -\boldsymbol{\xi}|\,\mathcal{O}\,|\boldsymbol{\xi}\rangle \tag{A.15}$$

In the following we summarize some equations regarding the expectation values in the coherent basis. The matrix element of a normal-ordered operator $\hat{\mathcal{O}}(c_i^\dagger, c_i)$ between two coherent states is very simple:

$$\langle\boldsymbol{\xi}|\,\hat{\mathcal{O}}(c_i, c_i^\dagger)\,|\boldsymbol{\xi}'\rangle = e^{\bar{\boldsymbol{\xi}}.\boldsymbol{\xi}'}\mathcal{O}(\xi_i', \bar{\xi}_i). \tag{A.16}$$

— B —

Appendix of Chapter 2

Example: XY-spin and Fermionic Hamiltonian comparison

Here, we are going to elaborate more on the computational implantation of XY model. We will discuss some examples with small sizes for a better demonstrarion.

A chain with two spins: In this example, we only consider two spins on a chain. The Hamiltonian of this system will be as below.

$$H = -J\Big(\frac{1+\gamma}{4}\sigma_1^x\sigma_2^x + \frac{1-\gamma}{4}\sigma_1^y\sigma_2^y\Big) - \frac{h}{2}\Big(\sigma_1^z + \sigma_2^z\Big) \tag{E.1.1.1}$$

It obvious that for only particles, we do not need to distinguish between open and periodic boundary conditions. This system has four states which in z-basis they would be $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$. Since, we are working in the z-basis, the Hamiltonan matrix would be

$$H = \begin{pmatrix} -h & 0 & 0 & -\frac{J\gamma}{2} \\ 0 & 0 & -\frac{J}{2} & 0 \\ 0 & -\frac{J}{2} & 0 & 0 \\ -\frac{J\gamma}{2} & 0 & 0 & h \end{pmatrix}$$

Next, we are going to diagonalize this Hamiltonian by solving the eigenvalue equation $\det[H - \lambda\mathbb{1}] = 0$. It will yield the following eigenvalues and the associated eigenvectors:

$$\lambda_i = \begin{cases} -\frac{J}{2} \\ \frac{J}{2} \\ -\frac{1}{2}\sqrt{\gamma^2J^2 + 4h^2} \\ \frac{1}{2}\sqrt{\gamma^2J^2 + 4h^2} \end{cases} \quad , \qquad |\lambda_i\rangle \to \begin{cases} \frac{1}{\sqrt{2}}|\downarrow\uparrow\rangle + \frac{1}{\sqrt{2}}|\uparrow\downarrow\rangle \\ \frac{1}{\sqrt{2}}|\downarrow\uparrow\rangle - \frac{1}{\sqrt{2}}|\uparrow\downarrow\rangle \\ \frac{J\gamma}{\sqrt{2c_\lambda(2h+c_\lambda)}}|\downarrow\downarrow\rangle + \sqrt{\frac{2h+c_\lambda}{2c_\lambda}}|\uparrow\uparrow\rangle \\ \frac{J\gamma}{\sqrt{2c_\lambda(c_\lambda-2h)}}|\downarrow\downarrow\rangle - \sqrt{\frac{c_\lambda-2h}{2c_\lambda}}|\uparrow\uparrow\rangle \end{cases} ;$$

where $c_\lambda = \sqrt{4h^2 + J^2\gamma^2}$.

A chain with three spins: Unlike the previous example, in this case we need to note the boundary conditions. Also, it is important to note the convention for ordering of rows (Columns) here. The below chosed ordering is based on the Mathematica's application ordering convention,

$$\begin{aligned} |1\rangle &= |\uparrow\uparrow\uparrow\rangle\,, \quad |2\rangle = |\uparrow\uparrow\downarrow\rangle\,, \quad |3\rangle = |\uparrow\downarrow\uparrow\rangle\,, \quad |4\rangle = |\uparrow\downarrow\downarrow\rangle \\ |5\rangle &= |\downarrow\uparrow\uparrow\rangle\,, \quad |6\rangle = |\downarrow\uparrow\downarrow\rangle\,, \quad |7\rangle = |\downarrow\downarrow\uparrow\rangle\,, \quad |8\rangle = |\downarrow\downarrow\downarrow\rangle \end{aligned} \tag{E.1.1.2}$$

Hamiltonian matrix for an open chain (in z-basis) is

$$H_{obc} = \begin{pmatrix} -\frac{3h}{2} & 0 & 0 & -\frac{J\gamma}{2} & 0 & 0 & -\frac{J\gamma}{2} & 0 \\ 0 & -\frac{h}{2} & -\frac{J}{2} & 0 & 0 & 0 & 0 & -\frac{J\gamma}{2} \\ 0 & -\frac{J}{2} & -\frac{h}{2} & 0 & -\frac{J}{2} & 0 & 0 & 0 \\ -\frac{J\gamma}{2} & 0 & 0 & \frac{h}{2} & 0 & -\frac{J}{2} & 0 & 0 \\ 0 & 0 & -\frac{J}{2} & 0 & -\frac{h}{2} & 0 & 0 & -\frac{J\gamma}{2} \\ 0 & 0 & 0 & -\frac{J}{2} & 0 & \frac{h}{2} & -\frac{J}{2} & 0 \\ -\frac{J\gamma}{2} & 0 & 0 & 0 & 0 & -\frac{J}{2} & \frac{h}{2} & 0 \\ 0 & -\frac{J\gamma}{2} & 0 & 0 & -\frac{J\gamma}{2} & 0 & 0 & \frac{3h}{2} \end{pmatrix}$$

Eigenvalues and eigenstates are as below (For sake of simplicity and as an attempt to not write complicated terms here we only write in symbolic terms!)

$$|E_1\rangle = \begin{pmatrix} 0 \\ -1 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad E_1 = -\frac{h}{2} \qquad |E_2\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad E_2 = \frac{h}{2} \qquad |E_3\rangle = \begin{pmatrix} 0 \\ \alpha_1 \\ \beta_1 \\ 0 \\ \delta_1 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad E_3 = \lambda_3$$

$$|E_4\rangle = \begin{pmatrix} 0 \\ \alpha_2 \\ \beta_2 \\ 0 \\ \delta_2 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad E_4 = \lambda_4 \qquad |E_5\rangle = \begin{pmatrix} 0 \\ \alpha_3 \\ \beta_3 \\ 0 \\ \delta_3 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad E_5 = \lambda_5 \qquad |E_6\rangle = \begin{pmatrix} \alpha_4 \\ 0 \\ 0 \\ 1 \\ 0 \\ \beta_4 \\ 1 \\ 0 \end{pmatrix}, \quad E_6 = \lambda_6$$

$$|E_7\rangle = \begin{pmatrix} \alpha_5 \\ 0 \\ 0 \\ 1 \\ 0 \\ \beta_5 \\ 1 \\ 0 \end{pmatrix}, \quad E_7 = \lambda_7 \qquad |E_8\rangle = \begin{pmatrix} \alpha_6 \\ 0 \\ 0 \\ 1 \\ 0 \\ \beta_6 \\ 1 \\ 0 \end{pmatrix}, \quad E_8 = \lambda_8$$

For the periodic boundary conditions, we have

$$H_{pbc} = \begin{pmatrix} \frac{-3h}{2} & 0 & 0 & \frac{-J\gamma}{2} & 0 & \frac{-J\gamma}{2} & \frac{-J\gamma}{2} & 0 \\ 0 & \frac{-h}{2} & \frac{-J}{2} & 0 & \frac{-J}{2} & 0 & 0 & \frac{-J\gamma}{2} \\ 0 & \frac{-J}{2} & \frac{-h}{2} & 0 & \frac{-J}{2} & 0 & 0 & \frac{-J\gamma}{2} \\ \frac{-J\gamma}{2} & 0 & 0 & \frac{h}{2} & 0 & \frac{-J}{2} & \frac{-J}{2} & 0 \\ 0 & \frac{-J}{2} & \frac{-J}{2} & 0 & \frac{-h}{2} & 0 & 0 & \frac{-J\gamma}{2} \\ \frac{-J\gamma}{2} & 0 & 0 & \frac{-J}{2} & 0 & \frac{h}{2} & \frac{-J}{2} & 0 \\ \frac{-J\gamma}{2} & 0 & 0 & \frac{-J}{2} & 0 & \frac{-J}{2} & \frac{h}{2} & 0 \\ 0 & \frac{-J\gamma}{2} & \frac{-J\gamma}{2} & 0 & \frac{-J\gamma}{2} & 0 & 0 & \frac{3h}{2} \end{pmatrix}$$

Eigenvalues and eigenstates for the PBC are

$$|E_1\rangle = \begin{pmatrix} 0 \\ -1 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad E_1 = \frac{J-h}{2} \qquad |E_2\rangle = \begin{pmatrix} 0 \\ -1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad E_2 = \frac{J-h}{2} \qquad |E_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad E_3 = \frac{J+h}{2}$$

$$|E_4\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad E_4 = \frac{J+h}{2} \qquad |E_5\rangle = \begin{pmatrix} \frac{2h-J+\alpha}{J\gamma} \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}, \quad E_5 = -\frac{h+J+\alpha}{2}$$

$$|E_6\rangle = \begin{pmatrix} \frac{2h-J-\alpha}{J\gamma} \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}, \quad E_6 = -\frac{h+J-\alpha}{2} \qquad |E_7\rangle = \begin{pmatrix} 0 \\ \frac{2h+J+J\gamma^2+\beta}{\gamma(-2h+2J+\beta)} \\ \frac{2h+J+J\gamma^2+\beta}{\gamma(-2h+2J+\beta)} \\ 0 \\ \frac{2h+J+J\gamma^2+\beta}{\gamma(-2h+2J+\beta)} \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad E_7 = \frac{h-J-\beta}{2}$$

$$|E_8\rangle = \begin{pmatrix} 0 \\ -\frac{2h+J+J\gamma^2-\beta}{\gamma(2h-2J+\beta)} \\ -\frac{2h+J+J\gamma^2-\beta}{\gamma(2h-2J+\beta)} \\ 0 \\ -\frac{2h+J+J\gamma^2-\beta}{\gamma(2h-2J+\beta)} \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad E_8 = \frac{h-J+\beta}{2}$$

In this part, we are going to compare the free fermionic Hamiltonian (2.34) with equation (2.2). For to fermions the fermionic Hamiltonian reads as

$$H_{XY} = \frac{J}{2}\left(c_1^\dagger c_2 + \gamma c_1^\dagger c_2^\dagger + c_2^\dagger c_1 + \gamma c_2 c_1\right) - h(c_1^\dagger c_1 + c_2^\dagger c_2) + h$$

For two particles, open and periodic boundary conditions have the same form. Before we proceed further, it is necessary to talk about the eigen-states of this two-body Hamiltonian. we start by XY-Hamiltonian eigen-state, $|\downarrow\downarrow\rangle = |00\rangle$ then $|\uparrow\downarrow\rangle = c_1^\dagger |00\rangle$, and consequently

$$\begin{aligned} |\downarrow\downarrow\rangle &= |00\rangle \\ |\downarrow\uparrow\rangle &= |01\rangle = -c_2^\dagger |00\rangle, \quad |\uparrow\downarrow\rangle = |10\rangle = c_1^\dagger |00\rangle \\ |\uparrow\uparrow\rangle &= |11\rangle = c_2^\dagger c_1^\dagger |00\rangle = -c_1^\dagger c_2^\dagger |00\rangle \end{aligned}$$

But why there is a mines sign? The reason is when we write $|1\cdots 1\rangle$ it means $c_1^\dagger|0\rangle\cdots c_n^\dagger|0\rangle$. So in a term like $c_n^\dagger\cdots c_1^\dagger$ acting on $|0\cdots 0\rangle$ we need to move the $c_{i>1}^\dagger$ to the right of c_1 and that produces some mines signs. Using this analogy and the same computation logic , matrix representation of the above equation is (not normalized!)

$$H_{XY} = -\frac{1}{2}\begin{pmatrix} 2h & 0 & 0 & J\gamma \\ 0 & 0 & J & 0 \\ 0 & J & 0 & 0 \\ J\gamma & 0 & 0 & -2h \end{pmatrix}$$

Eigenvalues and corresponding eigenvectors are as follow

$$|E_1\rangle = \frac{1}{\sqrt{2}}(\,|10\rangle + |01\rangle\,),\quad E_1 = -\frac{J}{2}\quad\text{and}\quad |E_2\rangle = \frac{1}{\sqrt{2}}(\,|01\rangle - |10\rangle\,),\quad E_2 = \frac{J}{2}$$

$$|E_3\rangle = \frac{2h+\lambda}{\gamma J}|11\rangle + |00\rangle\,,\quad E_3 = -\frac{\lambda}{2}$$

and

$$|E_4\rangle = \frac{2h-\lambda}{\gamma J}|11\rangle + |00\rangle\,,\quad E_4 = \frac{\lambda}{2}$$

where $\lambda = \sqrt{\gamma^2 J^2 + 4h^2}$. With these results, it is obvious that both these two-body Hamiltonians (before and after the fermionic transformation) have the same spectrum and eigen-states.

Next we will investigate the three body Hamiltonian (2.34) and compare the resulted eigenvalue and eigenvectors with those of the original XY Hamiltonian (2.2). In general, the fermionic Hamiltonian for three particles is

$$\begin{aligned} H_{XY} =& \frac{J}{2}\Big(c_1^\dagger c_2 + c_2^\dagger c_3 + \gamma c_1^\dagger c_2^\dagger + \gamma c_2^\dagger c_3^\dagger + c_2^\dagger c_1 + c_3^\dagger c_2 + \gamma c_2 c_1 + \gamma c_3 c_2\Big) \\ & - h(c_1^\dagger c_1 + c_2^\dagger c_2 + c_3^\dagger c_3) - \frac{J\mathcal{N}}{2}\Big(c_3^\dagger c_1 - c_3 c_1^\dagger + \gamma c_3^\dagger c_1^\dagger - \gamma c_3 c_1\Big) + \frac{3h}{2} \end{aligned}$$

which $\mathcal{N}$ determines the boundary condition. It is zero for open chain and ± 1 for periodic one. First we probe the open fermmionic chain which we have

$$H_O = \begin{pmatrix} -\frac{3h}{2} & 0 & 0 & -\frac{J\gamma}{2} & 0 & 0 & -\frac{J\gamma}{2} & 0 \\ 0 & -\frac{h}{2} & -\frac{J}{2} & 0 & 0 & 0 & 0 & -\frac{J\gamma}{2} \\ 0 & -\frac{J}{2} & -\frac{h}{2} & 0 & -\frac{J}{2} & 0 & 0 & 0 \\ -\frac{J\gamma}{2} & 0 & 0 & \frac{h}{2} & 0 & -\frac{J}{2} & 0 & 0 \\ 0 & 0 & -\frac{J}{2} & 0 & -\frac{h}{2} & 0 & 0 & -\frac{J\gamma}{2} \\ 0 & 0 & 0 & -\frac{J}{2} & 0 & \frac{h}{2} & -\frac{J}{2} & 0 \\ -\frac{J\gamma}{2} & 0 & 0 & 0 & 0 & -\frac{J}{2} & \frac{h}{2} & 0 \\ 0 & -\frac{J\gamma}{2} & 0 & 0 & -\frac{J\gamma}{2} & 0 & 0 & \frac{3h}{2} \end{pmatrix}$$

Eigenvalues and eigenstates are calculated in subsection 2.2.2 for this type of boundary.

Indeed, these calculation are much easier in the periodic boundary conditions. However, we should note that in the fermionic system periodic boundary can be a little tricky. for instance, $\mathcal{N} = \pm 1$ and that means we have two matrices for this boundary conditions.

$$H_P^{\mathcal{N}=+1} = \begin{pmatrix} -\frac{3h}{2} & 0 & 0 & -\frac{J\gamma}{2} & 0 & -\frac{J\gamma}{2} & -\frac{J\gamma}{2} & 0 \\ 0 & -\frac{h}{2} & -\frac{J}{2} & 0 & \frac{J}{2} & 0 & 0 & -\frac{J\gamma}{2} \\ 0 & -\frac{J}{2} & -\frac{h}{2} & 0 & -\frac{J}{2} & 0 & 0 & \frac{J\gamma}{2} \\ -\frac{J\gamma}{2} & 0 & 0 & \frac{h}{2} & 0 & -\frac{J}{2} & -\frac{J}{2} & 0 \\ 0 & \frac{J}{2} & -\frac{J}{2} & 0 & -\frac{h}{2} & 0 & 0 & -\frac{J\gamma}{2} \\ -\frac{J\gamma}{2} & 0 & 0 & -\frac{J}{2} & 0 & \frac{h}{2} & -\frac{J}{2} & 0 \\ -\frac{J\gamma}{2} & 0 & 0 & -\frac{J}{2} & 0 & -\frac{J}{2} & \frac{h}{2} & 0 \\ 0 & -\frac{J\gamma}{2} & \frac{J\gamma}{2} & 0 & -\frac{J\gamma}{2} & 0 & 0 & \frac{3h}{2} \end{pmatrix}$$

Eigenvalues and eigenstates are:

$$\left|E_1^+\right\rangle = \begin{pmatrix} 0 \\ -1 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad E_1^+ = -\frac{h+J}{2} \qquad \left|E_2^+\right\rangle = \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad E_2^+ = -\frac{h+J}{2} \qquad \left|E_3^+\right\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad E_3^+ = \frac{h+J}{2}$$

$$\left|E_4^+\right\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad E_4^+ = \frac{h+J}{2} \qquad \left|E_5^+\right\rangle = \begin{pmatrix} -\frac{J-2h-\alpha}{J\gamma} \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}, \quad E_5^+ = -\frac{J+h+\alpha}{2}$$

$$\left|E_6^+\right\rangle = \begin{pmatrix} 0 \\ \frac{2h-J-J\gamma^2+\alpha}{\gamma(2h+2J-\alpha)} \\ \frac{-2h+J+J\gamma^2-\alpha}{\gamma(2h+2J-\alpha)} \\ 0 \\ \frac{2h-J-J\gamma^2+\alpha}{\gamma(2h+2J-\alpha)} \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad E_6^+ = \frac{J+h-\alpha}{2} \qquad \left|E_7^+\right\rangle = \begin{pmatrix} \frac{2h-J-\alpha}{J\gamma} \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}, \quad E_7^+ = -\frac{J+h-\alpha}{2}$$

$$\left|E_8^+\right\rangle = \begin{pmatrix} 0 \\ \frac{2h-J-J\gamma^2-\alpha}{\gamma(2h+2J+\alpha)} \\ -\frac{2h-J-J\gamma^2-\alpha}{\gamma(2h+2J+\alpha)} \\ 0 \\ \frac{2h-J-J\gamma^2-\alpha}{\gamma(2h+2J)\alpha)} \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad E_8^+ = \frac{J+h+\alpha}{2}$$

Also for $\mathcal{N} = -1$ we have

$$H_P^{\mathcal{N}=-1} = \begin{pmatrix} -\frac{3h}{2} & 0 & 0 & -\frac{J\gamma}{2} & 0 & \frac{J\gamma}{2} & -\frac{J\gamma}{2} & 0 \\ 0 & -\frac{h}{2} & -\frac{J}{2} & 0 & -\frac{J}{2} & 0 & 0 & -\frac{J\gamma}{2} \\ 0 & -\frac{J}{2} & -\frac{h}{2} & 0 & -\frac{J}{2} & 0 & 0 & -\frac{J\gamma}{2} \\ -\frac{J\gamma}{2} & 0 & 0 & \frac{h}{2} & 0 & -\frac{J}{2} & \frac{J}{2} & 0 \\ 0 & -\frac{J}{2} & -\frac{J}{2} & 0 & -\frac{h}{2} & 0 & 0 & -\frac{J\gamma}{2} \\ \frac{J\gamma}{2} & 0 & 0 & -\frac{J}{2} & 0 & \frac{h}{2} & -\frac{J}{2} & 0 \\ -\frac{J\gamma}{2} & 0 & 0 & \frac{J}{2} & 0 & -\frac{J}{2} & \frac{h}{2} & 0 \\ 0 & -\frac{J\gamma}{2} & -\frac{J\gamma}{2} & 0 & -\frac{J\gamma}{2} & 0 & 0 & \frac{3h}{2} \end{pmatrix}$$

So the eigenvalues and eigenstates are

$$\left|E_1^-\right\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad E_1^- = \frac{h-J}{2} \qquad \left|E_2^-\right\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad E_2^- = \frac{h-J}{2} \qquad \left|E_3^-\right\rangle = \begin{pmatrix} 0 \\ -1 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad E_3^- = \frac{J-h}{2}$$

$$\left|E_4^-\right\rangle = \begin{pmatrix} 0 \\ -1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad E_4^- = \frac{J-h}{2} \qquad \left|E_5^-\right\rangle = \begin{pmatrix} 0 \\ \frac{2h+J+J\gamma^2+\beta}{\gamma(-2h+2J+\beta)} \\ \frac{2h+J+J\gamma^2+\beta}{\gamma(-2h+2J+\beta)} \\ 0 \\ \frac{2h+J+J\gamma^2+\beta}{\gamma(-2h+2J+\beta)} \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad E_5^- = \frac{h-J-\beta}{2}$$

$$\left|E_6^-\right\rangle = \begin{pmatrix} \frac{2h+J+\beta}{J\gamma} \\ 0 \\ 0 \\ 1 \\ 0 \\ -1 \\ 1 \\ 0 \end{pmatrix}, \quad E_6^- = \frac{J-h-\beta}{2} \qquad \left|E_7^-\right\rangle = \begin{pmatrix} 0 \\ -\frac{2h+J+J\gamma^2-\beta}{\gamma(2h-2J+\beta)} \\ -\frac{2h+J+J\gamma^2-\beta}{\gamma(2h-2J+\beta)} \\ 0 \\ -\frac{2h+J+J\gamma^2-\beta}{\gamma(2h-2J+\beta)} \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad E_7^- = \frac{h-J+\beta}{2}$$

$$\left|E_8^-\right\rangle = \begin{pmatrix} \frac{2h+J-\beta}{J\gamma} \\ 0 \\ 0 \\ 1 \\ 0 \\ -1 \\ 1 \\ 0 \end{pmatrix}, \quad E_8^- = \frac{-h+J+\beta}{2}$$

Where $\alpha = (4h^2 - 4hJ + J^2 + 3J^2\gamma^2)^{\frac{1}{2}}$ and $\beta = (4h^2 + 4hJ + J^2 + 3J^2\gamma^2)^{\frac{1}{2}}$.

This two Hamiltonian (periodic boundary condition) have sixteen eigenvalues and corresponding eigenstates. However, before the JW transformation, we had 8 eigenvalues with the same number of particles and boundary condition. It is necessary to identify which of these states are irrelevant, and to do so, we make a comparison with results of the same system before the JW transformation. To determine which eigenstates are favorable and which are not let us act on them with $\hat{\mathcal{N}}$.

$$\hat{\mathcal{N}}\left|E_i^+\right\rangle = \begin{cases} +\left|E_i^+\right\rangle & i = 3,4,5,7 \\ -\left|E_i^+\right\rangle & i = 1,2,6,8 \end{cases}$$

$$\hat{\mathcal{N}}\left|E_i^-\right\rangle = \begin{cases} +\left|E_i^-\right\rangle & i = 1,2,6,8 \\ -\left|E_i^-\right\rangle & i = 3,4,5,7 \end{cases}$$

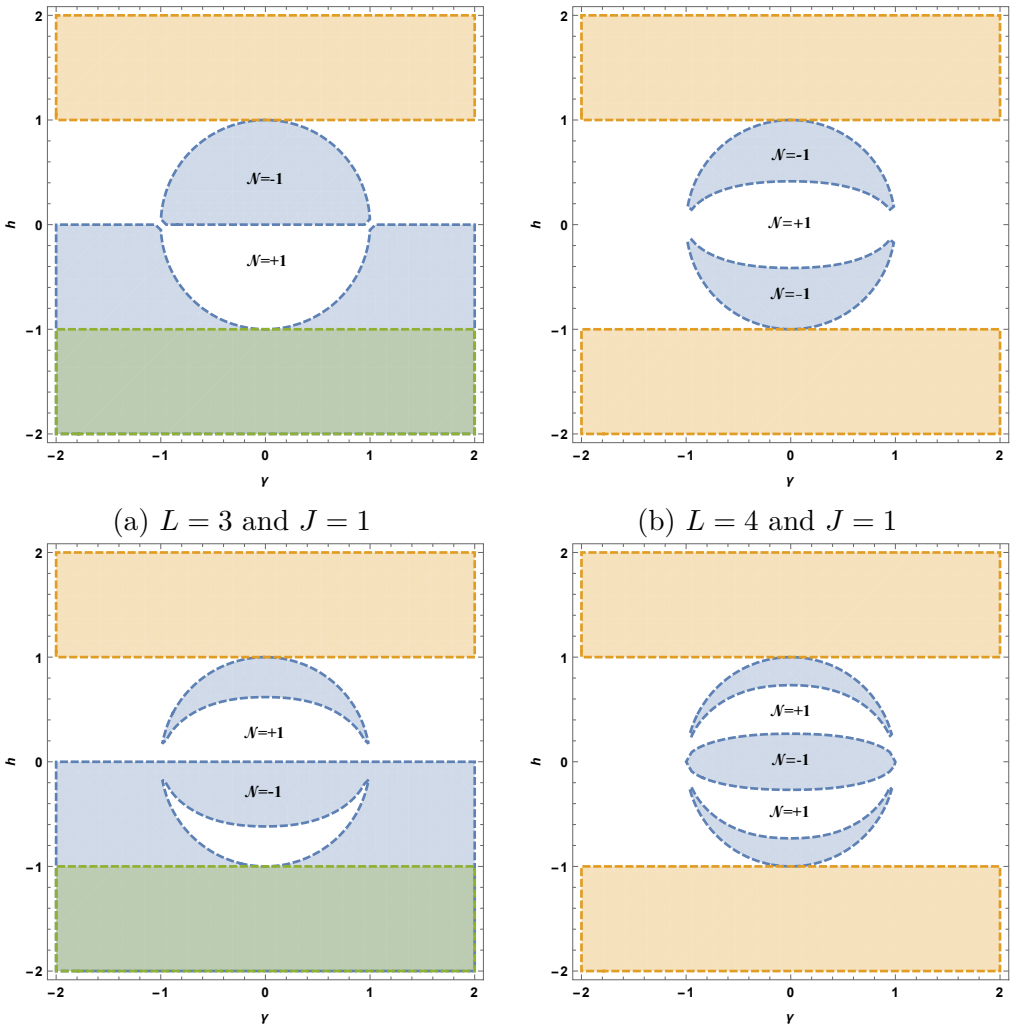
The logic behind the selection of relevant states is simple, we want those states which respect the Parity. For instance,

$$\hat{\mathcal{N}}\left|E_i^\pm\right\rangle = \pm\left|E_i^\pm\right\rangle \tag{B.1}$$

and the rest are unrelated.

Another question which needs to be addressed is that the real ground state lies in which sector of Hilbert space? The answer is it depends on the parameters. It can be seen by comparing the eigenvalues $E_i^\pm$ with those of periodic Hamiltonian in subsection 2.2.2, for $-1 < h < 1$, the ground state is alternatively lies in one of the $\mathcal{N} = \pm 1$ sectors. This mechanism is also called vacua competition between the two parity sectors (see figure 11). In this region, the first excited state is going to be the other sector's ground state ($\left|E_5^+\right\rangle$).

However, this is not the whole picture. By doing the same calculation for different number of particles and comparing the results of fermionic mapping with those of XY-model, an interesting case happens. For $h < -1$, the ground state with $\mathcal{N} = -1$ for even number of particles ($\mathcal{N} = +1$ for odd number of particles) is not physical because it has the wrong parity (B.1) and it is ruled out. Analogously, for $h > 1$ the ground state with $\mathcal{N} = -1$ for both even and odd number of particles is ruled out. We will elaborate on the phase transition in the XY-model and this change in ground state, later in this review. Aside from that, It is apparent that there is no specific order for states to be one from $\mathcal{N} = -1$ and the next one from the other sector. Never the less, half of them are from mines sector and the other half are from the positive sector.



(a) $L = 3$ and $J = 1$

(b) $L = 4$ and $J = 1$

(c) $L = 5$ and $J = 1$

(d) $L = 6$ and $J = 1$

Figure 11 – This is an illustration of different regions of XY-model phase diagram (also the fermionic system) for different L's. in the blue regions the real ground state lies in $\mathcal{N} = -1$ sector and white region for the other sector. In these regions both ground states of two sectors are physical. The orange (green) region corresponds to the case where $\mathcal{N} = -1$ ($\mathcal{N} = +1$) ground state or vacuum is not a physical state and, therefore, it does not appear in the XY spectrum. Graph is plotted for $J = 1$ and (a) $L = 3$, (b) $L = 4$, (c) $L = 5$ and (d) $L = 6$.

Details of calculations in section 2.2.5

Proof of commutation relations (2.31) from spin point of view.

$$\left\{c_l^\dagger, c_n^\dagger\right\} = \left\{\prod_{j<l}\sigma_j^z\sigma_l^+, \prod_{i<n}\sigma_i^z\sigma_n^+\right\} = \prod_{j<l}\sigma_j^z\sigma_l^+\prod_{i<n}\sigma_i^z\sigma_n^+ + \prod_{i<n}\sigma_i^z\sigma_n^+\prod_{j<l}\sigma_j^z\sigma_l^+ \tag{B.2}$$

If $n = l$ then $\prod\sigma_i^z\prod\sigma_i^z = 1$ and $\sigma_l^+\sigma_l^+ = 0$ so terms in the right side of the above equation vanishes. If $n \neq l$, then we assume that $n > l$. With this assumption, and using the fact that $\left\{\sigma_a^z, \sigma_b^+\right\} = 0$, in $\prod_{j<l}\sigma_j^z\sigma_l^+\prod_{i<n}\sigma_i^z\sigma_n^+$ we move σ_i^z to the left for all $i < l$. In the second term, $\prod_{i<n}\sigma_i^z\sigma_n^+\prod_{j<l}\sigma_j^z\sigma_l^+$, we move all the σ_j^z's to the left (they all commute with σ_n^+).

$$\left\{c_l^\dagger, c_n^\dagger\right\} = \sigma_l^+\prod_{i=l}^{n-1}\sigma_i^z\sigma_n^+ + \prod_{i=l}^{n-1}\sigma_i^z\sigma_n^+\sigma_l^+ = -\prod_{i=l}^{n-1}\sigma_i^z\sigma_l^+\sigma_n^+ + \prod_{i=l}^{n-1}\sigma_i^z\sigma_n^+\sigma_l^+ = 0 \tag{B.3}$$

Assuming $l > n$ would have resulted the same, although in that case we had to move σ_j^z to the right. Using the same procedure, we can show that $\{c_l, c_n\} = 0$. For the other anticommutation relation we have:

$$\begin{aligned}
\{c_l^\dagger, c_n\} =& \{\prod_{j<l}\sigma_j^z\sigma_l^+, \prod_{i<n}\sigma_i^z\sigma_n^-\} = \prod_{j<l}\sigma_j^z\sigma_l^+\prod_{i<n}\sigma_i^z\sigma_n^- + \prod_{i<n}\sigma_i^z\sigma_n^-\prod_{j<l}\sigma_j^z\sigma_l^+ \\
&\text{If} \quad n = l: \\
=& \prod_{j<l}\sigma_j^z\prod_{i<n}\sigma_i^z\sigma_l^+\sigma_n^- + \prod_{i<n}\sigma_i^z\prod_{j<l}\sigma_j^z\sigma_n^-\sigma_l^+ = \prod_i(\sigma_i^z)^2[\sigma_n^+\sigma_n^- + \sigma_n^-\sigma_n^+] = \mathbb{1} \\
&\text{IF} \quad n \neq l: \\
=& \prod_{i=l}^{n-1}\sigma_l^+\sigma_i^z\sigma_n^- + \prod_{i=l}^{n-1}\sigma_i^z\sigma_n^-\sigma_l^+ = -\prod_{i=l}^{n-1}\sigma_i^z\sigma_l^+\sigma_n^- + \prod_{i=l}^{n-1}\sigma_i^z\sigma_n^-\sigma_l^+ = 0
\end{aligned} \tag{B.4}$$

Therefore, we have $\{c_l^\dagger, c_n\} = \delta_{n,l}$.

$$
\begin{aligned}
\Big[\hat{\mathcal{N}}, H_{XY}\Big] &= -J[\prod_{n=1}^{L}\sigma_n^z, \sum_{l=1}^{L}\Big(\frac{1+\gamma}{4}\sigma_l^x\sigma_{l+1}^x + \frac{1-\gamma}{4}\sigma_l^y\sigma_{l+1}^y\Big)] \\
&= \sum_l \frac{1+\gamma}{4}[\prod_n \sigma_n^z, \sigma_l^x\sigma_{l+1}^x] + \sum_l \frac{1-\gamma}{4}[\prod_n \sigma_n^z, \sigma_l^y\sigma_{l+1}^y] \\
&= \sum_l \frac{1+\gamma}{4}[\prod_n \sigma_n^z, \sigma_l^x]\sigma_{l+1}^x + \sum_l \frac{1+\gamma}{4}\sigma_l^x[\prod_n \sigma_n^z, \sigma_{l+1}^x] \\
&\quad + \sum_l \frac{1-\gamma}{4}\sigma_l^y[\prod_n \sigma_n^z, \sigma_{l+1}^y] + \sum_l \frac{1-\gamma}{4}[\prod_n \sigma_n^z, \sigma_l^y]\sigma_{l+1}^y \\
&= \sum_l \frac{1+\gamma}{4}\sigma_l'^z[\sigma_l^z, \sigma_l^x]\sigma_{l+1}^x + \sum_l \frac{1+\gamma}{4}\sigma_l^x\sigma_{l+1}'^z[\sigma_{l+1}^z, \sigma_{l+1}^x] \\
&\quad + \sum_l \frac{1-\gamma}{4}\sigma_l^y\sigma_{l+1}'^z[\sigma_{l+1}^z, \sigma_{l+1}^y] + \sum_l \frac{1-\gamma}{4}\sigma_l'^z[\sigma_l^z, \sigma_l^y]\sigma_{l+1}^y \\
&= \sum_l i\frac{1+\gamma}{4}\sigma_{l,l+1}'^z\Big(\sigma_l^y\sigma_{l+1}^z\sigma_{l+1}^x + \sigma_l^x\sigma_l^z\sigma_{l+1}^y\Big) \\
&\quad - \sum_l i\frac{1-\gamma}{4}\sigma_{l,l+1}'^z\Big(\sigma_l^x\sigma_{l+1}^z\sigma_{l+1}^y + \sigma_l^y\sigma_l^z\sigma_{l+1}^x\Big) \\
&= -\sum_l \frac{1+\gamma}{4}\sigma_{l,l+1}'^z\Big(\sigma_l^y\sigma_{l+1}^y - \sigma_l^y\sigma_{l+1}^y\Big) + \sum_l \frac{1-\gamma}{4}\sigma_{l,l+1}'^z\Big(\sigma_l^x\sigma_{l+1}^x - \sigma_l^x\sigma_{l+1}^x\Big) = 0
\end{aligned}
\tag{B.5}
$$

where $\sigma_{l,l+1}'^z = \prod_{\substack{n=1\\ n\neq l,l+1}}^{L}\sigma_n^z$ and in the last line we have used the relation $\sigma^a\sigma^b = \delta_{a,b} + i\varepsilon_{abc}\sigma^c$.

Here, we go through the fermionization calculations part by part, using the relations (2.31) and (2.33). For start, let us transform the second part of the XY Hamiltonian (2.2).

$$
\frac{h}{2}\sum_{l=1}^{L}\sigma_l^z = \frac{h}{2}\sum_{l=1}^{L}(c_l^\dagger c_l - c_l c_l^\dagger) = \frac{h}{2}\sum_{l=1}^{L}(2c_l^\dagger c_l - 1) = h\sum_{l=1}^{L}c_l^\dagger c_l - \frac{hL}{2}
$$

For the interaction parts, we replace $\sigma_l^x\sigma_{l+1}^x = (c_l - c_l^\dagger)(c_{l+1} + c_{l+1}^\dagger)$ and $\sigma_l^y\sigma_{l+1}^y = -(c_l^\dagger + c_l)(c_{l+1} - c_{l+1}^\dagger)$. However, we should be very careful about the boundary. First, we only calculate this transformation up to site $L-1$,

$$
\begin{aligned}
\frac{J}{2}\sum_{l=1}^{L-1}\Big[\frac{1+\gamma}{2}\sigma_l^x\sigma_{l+1}^x + \frac{1-\gamma}{2}\sigma_l^y\sigma_{l+1}^y\Big] &= -\frac{J}{2}\sum_{l=1}^{L-1}\Big[\frac{1+\gamma}{2}(c_l^\dagger - c_l)(c_{l+1} + c_{l+1}^\dagger) \\
&\quad + \frac{1-\gamma}{2}(c_l^\dagger + c_l)(c_{l+1} - c_{l+1}^\dagger)\Big] = \frac{-J}{2}\sum_{l=1}^{L-1}\Big[c_l^\dagger c_{l+1} - c_l c_{l+1}^\dagger + \gamma c_l^\dagger c_{l+1}^\dagger - \gamma c_l c_{l+1}\Big].
\end{aligned}
$$

Now for the boundary sites L and 1 we have:

$$
\begin{aligned}
\frac{J}{2}\Big(\frac{1+\gamma}{2}\sigma_L^x\sigma_{L+1}^x + \frac{1-\gamma}{2}\sigma_L^y\sigma_{L+1}^y\Big) &= \frac{J}{2}\Big(\frac{1+\gamma}{2}\sigma_L^x\sigma_1^x + \frac{1-\gamma}{2}\sigma_L^y\sigma_1^y\Big) \\
&= \frac{J}{2}\Big[\frac{1+\gamma}{2}\prod_{j<L}\sigma_j^z(c_L^\dagger + c_L)(c_1 + c_1^\dagger) - \frac{1-\gamma}{2}\prod_{j<L}(c_L - c_L^\dagger)(c_1 - c_1^\dagger)\Big] \\
&= \frac{J\hat{\mathcal{N}}}{2}\Big[\frac{1+\gamma}{2}\sigma_L^z(c_L^\dagger + c_L)(c_1 + c_1^\dagger) - \frac{1-\gamma}{2}\sigma_L^z(c_L - c_L^\dagger)(c_1 - c_1^\dagger)\Big] \\
&= \frac{J\hat{\mathcal{N}}}{2}\Big[c_L^\dagger c_1 + c_1^\dagger c_L + \gamma c_L^\dagger c_1^\dagger - \gamma c_L c_1\Big].
\end{aligned}
$$

In the third line we have used the relations $\sigma_L^z c_L^\dagger = c_L^\dagger$ and $\sigma_L^z c_L = -c_L$. Due to interchange of $\hat{\mathcal{N}}$ with c_L and $c_l^\dagger$ a minus sign is also produced, $\left\{\hat{\mathcal{N}}, c_l^{(\dagger)}\right\} = 0$, which shows that this Hamiltonian is Hermitian.

XY model symmetry and transformation calculation

$$\begin{aligned} A_{XX} =& \frac{1}{4}\Big[(\gamma+1)\sin^4(\alpha)n_x^4 + 2\sin^2(\alpha)n_x^2\Big((1-3\gamma)\sin^2(\alpha)n_y^2 + (\gamma+1) \\ & \times [\cos^2(\alpha) - \sin^2(\alpha)n_z^2]\Big) - 8(\gamma-1)\sin^3(\alpha)\cos(\alpha)n_x n_y n_z \\ & + (\gamma+1)\left(\cos^2(\alpha) - \sin^2(\alpha)n_y^2\right)^2 + 2\sin^2(\alpha)n_z^2[(1-3\gamma)\cos^2(\alpha) \\ & + (\gamma+1)\sin^2(\alpha)n_y^2] + (\gamma+1)\sin^4(\alpha)n_z^4\Big] \end{aligned} \tag{B.6}$$

$$\begin{aligned} A_{YY} =& -\frac{1}{4}\gamma\cos^4(\alpha) + \frac{\cos^4(\alpha)}{4} - \frac{1}{4}\gamma\sin^4(\alpha)n_x^4 + \frac{1}{2}\gamma\sin^2(\alpha)\cos^2(\alpha)n_x^2 \\ & + \frac{1}{4}\sin^4(\alpha)n_x^4 - \frac{1}{2}\sin^2(\alpha)\cos^2(\alpha)n_x^2 + \frac{3}{2}\gamma\sin^4(\alpha)n_x^2 n_y^2 \\ & + \frac{1}{2}\sin^4(\alpha)n_x^2 n_y^2 - 2\gamma\sin^3(\alpha)\cos(\alpha)n_x n_y n_z - 2\sin^3(\alpha)\cos(\alpha)n_x n_y n_z \\ & - \frac{1}{2}\gamma\sin^4(\alpha)n_x^2 n_z^2 + \frac{1}{2}\sin^4(\alpha)n_x^2 n_z^2 - \frac{1}{4}\gamma\sin^4(\alpha)n_y^4 \\ & - \frac{\gamma}{2}\sin^2(\alpha)\cos^2(\alpha)n_y^2 + \frac{1}{4}\sin^4(\alpha)n_y^4 + \frac{1}{2}\sin^2(\alpha)\cos^2(\alpha)n_y^2 \\ & + \frac{1}{2}\gamma\sin^4(\alpha)n_y^2 n_z^2 - \frac{1}{2}\sin^4(\alpha)n_y^2 n_z^2 - \frac{1}{4}\gamma\sin^4(\alpha)n_z^4 \\ & + \frac{3}{2}\gamma\sin^2(\alpha)\cos^2(\alpha)n_z^2 + \frac{1}{4}\sin^4(\alpha)n_z^4 + \frac{1}{2}\sin^2(\alpha)\cos^2(\alpha)n_z^2 \end{aligned} \tag{B.7}$$

$$\begin{aligned} A_{ZZ} =& -\gamma\sin^2(\alpha)\cos^2(\alpha)n_x^2 + \sin^2(\alpha)\cos^2(\alpha)n_x^2 + 4\gamma\sin^3(\alpha)\cos(\alpha)n_x n_y n_z \\ & + \gamma\sin^4(\alpha)n_x^2 n_z^2 + \sin^4(\alpha)n_x^2 n_z^2 + \gamma\sin^2(\alpha)\cos^2(\alpha)n_y^2 \\ & + \sin^2(\alpha)\cos^2(\alpha)n_y^2 - \gamma\sin^4(\alpha)n_y^2 n_z^2 + \sin^4(\alpha)n_y^2 n_z^2 \end{aligned} \tag{B.8}$$

$$\begin{aligned} A_{XY} = A_{YX} =& -\gamma\sin^4(\alpha)n_x n_y^3 + \gamma\sin^4(\alpha)n_x^3 n_y + \sin^2(\alpha)\cos^2(\alpha)n_x n_y \\ & - \sin^4(\alpha)n_x n_y n_z^2 - \sin^3(\alpha)\cos(\alpha)n_x^2 n_z + \sin^3(\alpha)\cos(\alpha)n_y^2 n_z \\ & - \gamma\sin(\alpha)\cos^3(\alpha)n_z + \gamma\sin^3(\alpha)\cos(\alpha)n_z^3 \end{aligned} \tag{B.9}$$

$$
\begin{aligned}
A_{XZ} = A_{ZX} =& \frac{3}{2}\gamma \sin^3(\alpha)\cos(\alpha)n_x^2 n_y - \frac{1}{2}\sin^3(\alpha)\cos(\alpha)n_x^2 n_y \\
&- \frac{3}{2}\gamma \sin^4(\alpha)n_x n_y^2 n_z + \frac{1}{2}\sin^4(\alpha)n_x n_y^2 n_z - \frac{1}{2}\gamma \sin^4(\alpha)n_x n_z^3 \\
&+ \frac{1}{2}\gamma \sin^4(\alpha)n_x^3 n_z + \frac{3}{2}\gamma \sin^2(\alpha)\cos^2(\alpha)n_x n_z - \frac{1}{2}\sin^4(\alpha)n_x n_z^3 \\
&+ \frac{1}{2}\sin^4(\alpha)n_x^3 n_z - \frac{1}{2}\sin^2(\alpha)\cos^2(\alpha)n_x n_z + \frac{1}{2}\gamma \sin(\alpha)\cos^3(\alpha)n_y \\
&- \frac{1}{2}\gamma \sin^3(\alpha)\cos(\alpha)n_y^3 + \frac{1}{2}\sin(\alpha)\cos^3(\alpha)n_y - \frac{1}{2}\sin^3(\alpha)\cos(\alpha)n_y^3 \\
&- \frac{3}{2}\gamma \sin^3(\alpha)\cos(\alpha)n_y n_z^2 + \frac{1}{2}\sin^3(\alpha)\cos(\alpha)n_y n_z^2
\end{aligned}
\tag{B.10}
$$

$$
\begin{aligned}
A_{YZ} = A_{ZY} =& \frac{1}{2}\gamma \sin(\alpha)\cos^3(\alpha)n_x - \frac{1}{2}\gamma \sin^3(\alpha)\cos(\alpha)n_x^3 \\
&- \frac{1}{2}\sin(\alpha)\cos^3(\alpha)n_x + \frac{1}{2}\sin^3(\alpha)\cos(\alpha)n_x^3 \\
&+ \frac{3}{2}\gamma \sin^3(\alpha)\cos(\alpha)n_x n_y^2 + \frac{1}{2}\sin^3(\alpha)\cos(\alpha)n_x n_y^2 \\
&+ \frac{3}{2}\gamma \sin^4(\alpha)n_x^2 n_y n_z + \frac{1}{2}\sin^4(\alpha)n_x^2 n_y n_z - \frac{3}{2}\gamma \sin^3(\alpha)\cos(\alpha)n_x n_z^2 \\
&- \frac{1}{2}\sin^3(\alpha)\cos(\alpha)n_x n_z^2 + \frac{1}{2}\gamma \sin^4(\alpha)n_y n_z^3 - \frac{1}{2}\gamma \sin^4(\alpha)n_y^3 n_z \\
&- \frac{3}{2}\gamma \sin^2(\alpha)\cos^2(\alpha)n_y n_z - \frac{1}{2}\sin^4(\alpha)n_y n_z^3 + \frac{1}{2}\sin^4(\alpha)n_y^3 n_z \\
&- \frac{1}{2}\sin^2(\alpha)\cos^2(\alpha)n_y n_z
\end{aligned}
\tag{B.11}
$$

$$
B_X = 2n_x n_z \sin[2](\alpha) - 2n_y \cos(\alpha)\sin(\alpha) \tag{B.12}
$$

$$
B_Y = 2n_y n_z \sin[2](\alpha) + 2n_x \cos(\alpha)\sin(\alpha) \tag{B.13}
$$

$$
B_Z = \cos[2](\alpha) + (n_z^2 - n_x^2 - n_y^2)\sin[2](\alpha) \tag{B.14}
$$

Example: Identification of spin chain spectrum after fermionization

Example: Let us consider an example of this Bogoliubov form of XY Hamiltonian and compare the outcome with the results of appendix B and 2.2.2. In particular, we consider the case with $L = 3$ in the weak field region. Therefore, $k = 1, 2, 3$, also, we first look at the $\mathcal{N} = +1$.

$$
\phi_1^+ = \tfrac{\pi}{3} \quad \lambda_1^+ = \tfrac{1}{2}\sqrt{J^2 - 4Jh + 4h^2 + 3J^2\gamma^2}
$$

$$
\phi_2^+ = \pi \quad \lambda_2^+ = (J + h)
$$

$$
\phi_3^+ = \tfrac{5\pi}{3} \quad \lambda_3^+ = \tfrac{1}{2}\sqrt{J^2 - 4Jh + 4h^2 + 3J^2\gamma^2}
$$

For $\mathcal{N} = -1$ sector:

$$\phi_1^- = \tfrac{2\pi}{3} \quad \lambda_1^- = \tfrac{1}{2}\sqrt{J^2 + 4Jh + 4h^2 + 3J^2\gamma^2}$$

$$\phi_2^- = \tfrac{4\pi}{3} \quad \lambda_2^- = \tfrac{1}{2}\sqrt{J^2 + 4Jh + 4h^2 + 3J^2\gamma^2}$$

$$\phi_3^- = 2\pi \quad \lambda_3^- = (J - h)$$

Now, the ground state energy calculated via the b_k vacuum ($b_k \left|0\right\rangle_b = 0, \ \ \forall k$).

$$E_G^+ = -\frac{1}{2}(\lambda_1^+ + \lambda_2^+ + \lambda_3^+) = -\frac{J + h + \alpha}{2}$$
$$E_G^- = -\frac{1}{2}(\lambda_1^- + \lambda_2^- + \lambda_3^-) = -\frac{J - h + \beta}{2}$$

where $\alpha = \sqrt{J^2 - 4Jh + 4h^2 + 3J^2\gamma^2}$ and $\beta = \sqrt{J^2 + 4Jh + 4h^2 + 3J^2\gamma^2}$. These are the same as ground states calculated in the appendix B for the $L = 3$ (both sectors), namely $E_G^- = E_5^-$ and $E_G^+ = E_5^+$. In addition, both of these ground states do appear in the spectrum of the example XY spin Hamiltonians in section 2.2.2. For each sector, the first excited state is the $b_i^\dagger \left|0\right\rangle$ where $b_i^\dagger$ is the fermionic creation operator with $\lambda_i = \min[\lambda_k]$. For example, in $\mathcal{N} = -1$ sector, $\lambda_3^- < \lambda_1^- = \lambda_2^-$. Therefore the first excited state in this sector is $b_3^\dagger \left|0\right\rangle$ with energy $E_1 = -\frac{\lambda_1^- + \lambda_2^- + \lambda_3^-}{2} + \frac{\lambda_3^-}{2}$. The same logic works for the rest of spectrum. Equivalently, we can construct the spectrum in both sectors but states with $b_k^\dagger b_{k'}^\dagger \left|0\right\rangle_b$ ($k \neq k'$) are physical.

— C —

Appendix of Chapter 6

In the next three Appendices for the sake of completeness, we summarize first the spin chain version of the fermionic integrals of motion that we introduced in the main text. Then we introduce the method of correlations that can be used to calculate the entanglement entropy in the free fermions. In the third subsection, we comment on the degeneracies in the XX-chain and various averagings on the entanglement entropy of the excited states.

Integrals of motion: spin chains

This section serves to pay more attention to the spin version of the integrals of motion and the fermionic Hamiltonian defined in the main text. In most of the cases, the integrals of motion do not have a simple form. However, one can still claim that the Hamiltonian I_m^- which is parameter independent in the spin version, commutes with all the possible Hamiltonians and integrals of motion and so it provides bases which in those bases the average of entanglement entropy is equal for the eigenstates of I_m^- and the Hamiltonian. We begin by writing the spin form of fermionic operators using the Jordan-Wigner transformation

$$c_j = \prod_{l<j} \sigma_l^z \sigma_j^- . \tag{C.1}$$

where $\sigma_i^{\pm} = \frac{\sigma_i^x \pm \sigma_i^y}{2}$. Substituting the above in the fermionic Hamiltonian we get

$$\begin{aligned} H = & \sum_{r>0} \sum_{j=1}^{L-1} \Big[\frac{-a_r - b_r}{2} \sigma_j^x \sigma_{j+1}^z \cdots \sigma_{j+r-1}^z \sigma_{j+r}^x \\ & + \frac{-a_r + b_r}{2} \sigma_j^y \sigma_{j+1}^z \cdots \sigma_{j+r-1}^z \sigma_{j+r}^y \Big] - \sum_{j=1}^{L} \frac{a_0}{2} (\sigma_j^z - 1) \\ & - \hat{\mathcal{N}} \Big(\frac{-a_r - b_r}{2} \sigma_L^x \sigma_1^z \cdots \sigma_{r-1}^z \sigma_r^x \\ & + \frac{-a_r + b_r}{2} \sigma_L^y \sigma_1^z \cdots \sigma_{r-1}^z \sigma_r^y \Big), \end{aligned} \tag{C.2}$$

where $\hat{\mathcal{N}} = \prod_{l=1}^{L} \sigma_l^z$, is the parity of the spins down, i.e. the parity of the number of fermions. Because of the string of σ^z, the JW transformation is non-local. The non-locality of the JW transformation affects the boundary conditions through appearance of the operator $\hat{\mathcal{N}}$. The eigenvalues: $\mathcal{N} = +1$ and -1 correspond to anti-periodic and periodic boundary conditions respectively. The operator $\hat{\mathcal{N}}$ should appear every time we go from spin format to fermion format or vice versa. For instance, in the periodic boundary condition, one gets:

$$\begin{aligned} H(\mathcal{N}=-1) = & \sum_{r>0} \sum_{j=1}^{L} \Big[\frac{-a_r - b_r}{2} \sigma_j^x \sigma_{j+1}^z \cdots \sigma_{j+r-1}^z \sigma_{j+r}^x \\ & + \frac{-a_r + b_r}{2} \sigma_j^y \sigma_{j+1}^z \cdots \sigma_{j+r-1}^z \sigma_{j+r}^y \Big] \\ & - \sum_{j=1}^{L} \frac{a_0}{2} (\sigma_j^z - 1). \end{aligned} \tag{C.3}$$

The above Hamiltonian when a_r and b_r are nonzero just for $r = 0, 1$ becomes:

$$\begin{aligned} H_{r=0,\pm1}(\mathcal{N}=-1) = -\frac{a_1}{2}\sum_{j=1}^{L}\Big[(1+\frac{b_1}{a_1})\sigma_j^x\sigma_{j+1}^x \\ +(1-\frac{b_1}{a_1})\sigma_j^y\sigma_{j+1}^y\Big] - \frac{a_0}{2}\sum_{j=1}^{L}\sigma_j^z + \frac{La_0}{2}, \end{aligned} \tag{C.4}$$

which is the Hamiltonian of the anisotropic periodic XY spin chain with $-a_1 \mp b_1 = \frac{J(1\pm\gamma)}{2}$ and $a_0 = h$.

For Integrals of motion I_n^+ and I_m^-, we can find the spin form likewise. Using the inverse Fourier transformation, we write them in the c-fermion form. The c-fermion form of I_m^- is already written in the main text; therefore, the spin form of this operator is

$$I_m^- = -\frac{1}{4}\sum_{j=1}^{L-1}[\sigma_j^x\prod_{l=j+1}^{j+m-1}\sigma_l^z\sigma_{j+m}^y - \sigma_j^y\prod_{l=j+1}^{j+m-1}\sigma_l^z\sigma_{j+m}^x] + \frac{\hat{\mathcal{N}}}{4}[\sigma_L^x\prod_{l<m}\sigma_l^z\sigma_m^y - \sigma_L^y\prod_{l<m}\sigma_l^z\sigma_m^x]. \tag{C.5}$$

Putting $\mathcal{N} = -1$, the boundary term absorbs in the sum and I_m^- reads as:

$$I_m^-(\mathcal{N}=-1) = -\frac{1}{4}\sum_{j=1}^{L}\Big[\sigma_j^x\prod_{l=j+1}^{j+m-1}\sigma_l^z\sigma_{j+m}^y - \sigma_j^y\prod_{l=j+1}^{j+m-1}\sigma_l^z\sigma_{j+m}^x\Big]. \tag{C.6}$$

For I_n^+, the fermionic form would be

$$I_n^+ = \sum_{j\in\Lambda}\sum_{r=-R}^{R}\Big(\frac{a_r}{2}\Big[c_j^\dagger c_{j+r+n} + c_{j+n}^\dagger c_{j+r}\Big] + \frac{b_r}{4}\Big[c_j^\dagger c_{j+r+n}^\dagger + c_{j+n}^\dagger c_{j+r}^\dagger - c_j c_{j+n+r} - c_{j+n}c_{j+r}\Big]\Big). \tag{C.7}$$

In the XY spin chain case this integral of motion can be written as

$$\begin{aligned} I_{r=0,\pm1}^+ = \sum_{j\in\Lambda}\Big(\frac{J}{4}\Big[c_j^\dagger c_{j+n+1} + c_{j+n}^\dagger c_{j+1} + c_{j+1}^\dagger c_{j+n} + c_{j+n+1}^\dagger c_j\Big] + \frac{h}{2}\Big[c_j^\dagger c_{j+n} + c_{j+n}^\dagger c_j\Big] \\ + \frac{J\gamma}{4}\Big[c_j^\dagger c_{j+n+1}^\dagger + c_{j+n}^\dagger c_{j+1}^\dagger - c_j c_{j+n+1} - c_{j+n}c_{j+1}\Big]\Big), \end{aligned} \tag{C.8}$$

where we have used the fact that $a_r = a_{-r}$ and $b_r = -b_{-r}$. I_n^+ commutes with both the Hamiltonian (C.4) and I_m^-. To write the above expression in the spin form, we need to separate two possible cases: $n > 1$ and $n = 1$. Consequently, using the transformation (C.1), the spin form of integrals of motion is:

$$
\begin{aligned}
I^{+}_{r=0,\pm1} =& -J\sum_{j=1}^{L-n-1}\Big[\tfrac{(1+\gamma)}{8}\sigma^x_j\sigma^z_{j+1}\cdots\sigma^z_{j+n}\sigma^x_{j+n+1}+\tfrac{(1-\gamma)}{8}\sigma^y_j\sigma^z_{j+1}\cdots\sigma^z_{j+n}\sigma^y_{j+n+1}\Big]\\
&-J\sum_{j=1}^{L-n+1}\Big[\tfrac{(1-\gamma)}{8}\sigma^x_j\sigma^z_{j+1}\cdots\sigma^z_{j+n-2}\sigma^x_{j+n-1}+\tfrac{(1+\gamma)}{8}\sigma^y_j\sigma^z_{j+1}\cdots\sigma^z_{j+n-2}\sigma^y_{j+n-1}\Big]\\
&-\frac{h}{4}\sum_{j=1}^{L-n}\Big[\sigma^x_j\sigma^z_{j+1}\cdots\sigma^z_{j+n-1}\sigma^x_{j+n}+\sigma^y_j\sigma^z_{j+1}\cdots\sigma^z_{j+n-1}\sigma^y_{j+n}\Big] \qquad n>1\\
&+J\hat{\mathcal{N}}\sum_{j=L-n}^{L}\Big[\tfrac{(1+\gamma)}{8}\sigma^x_j\sigma^z_{j+1}\cdots\sigma^z_{j+n}\sigma^x_{j+n+1}+\tfrac{(1-\gamma)}{8}\sigma^y_j\sigma^z_{j+1}\cdots\sigma^z_{j+n}\sigma^y_{j+n+1}\Big]\\
&+J\hat{\mathcal{N}}\sum_{j=L-n+2}^{L}\Big[\tfrac{(1-\gamma)}{8}\sigma^x_{j+1}\sigma^z_{j+2}\cdots\sigma^z_{j+n-1}\sigma^x_{j+n}+\tfrac{(1+\gamma)}{8}\sigma^y_{j+1}\sigma^z_{j+2}\cdots\sigma^z_{j+n-1}\sigma^y_{j+n}\Big]\\
&+\frac{h\hat{\mathcal{N}}}{4}\sum_{j=L-n+1}^{L}\Big[\sigma^x_j\sigma^z_{j+1}\cdots\sigma^z_{j+n-1}\sigma^x_{j+n}+\sigma^y_j\sigma^z_{j+1}\cdots\sigma^z_{j+n-1}\sigma^y_{j+n}\Big],
\end{aligned}
\tag{C.9}
$$

$$
\begin{aligned}
I^{+}_{r=0,\pm1} =& -J\sum_{j=1}^{L-2}\Big[\tfrac{1+\gamma}{8}\sigma^x_j\sigma^z_{j+1}\sigma^x_{j+2}+\tfrac{1-\gamma}{8}\sigma^y_j\sigma^z_{j+1}\sigma^y_{j+2}\Big]-\frac{h}{4}\sum_{j=1}^{L-1}\Big[\sigma^x_j\sigma^x_{j+1}+\sigma^y_j\sigma^y_{j+1}\Big]+\frac{J}{4}\sum_{j\in\Lambda}\sigma^z_j\\
&+\hat{\mathcal{N}}J\Big[\tfrac{1+\gamma}{8}\sigma^x_{L-1}\sigma^z_L\sigma^x_1+\tfrac{1-\gamma}{8}\sigma^y_{L-1}\sigma^z_L\sigma^y_1+\tfrac{1+\gamma}{8}\sigma^x_L\sigma^z_1\sigma^x_2+\tfrac{1-\gamma}{8}\sigma^y_L\sigma^z_1\sigma^z_2\Big]\\
&+\frac{\hat{\mathcal{N}}h}{4}\Big[\sigma^x_L\sigma^x_1+\sigma^y_L\sigma^y_1\Big], \qquad n=1.
\end{aligned}
\tag{C.10}
$$

These quantities commute with each other and the Hamiltonian. Note that these operators commute with each other after fixing the $\mathcal{N}$ too. For example, with $R=1$, we have:

$$\Big[H_{r=0,\pm1}(\mathcal{N}=-1),I^{+}_{r=0,\pm1}(\mathcal{N}=-1)\Big]=0, \tag{C.11}$$

$$\Big[H_{r=0,\pm1}(\mathcal{N}=-1),I^{-}_{r=0,\pm1}(\mathcal{N}=-1)\Big]=0, \tag{C.12}$$

$$\Big[I^{-}_{r=0,\pm1}(\mathcal{N}=-1),I^{+}_{r=0,\pm1}(\mathcal{N}=-1)\Big]=0. \tag{C.13}$$

In a general case of R, we write for I^{+}_{n}:

$$
\begin{aligned}
I^{+}_{n} =& \sum_{r=-R}^{R}\Bigg[\sum_{j=1}^{L-n-r}\Big[\tfrac{(a_r+b_r)}{4}\sigma^x_j\sigma^z_{j+1}\cdots\sigma^z_{j+n+r-1}\sigma^x_{j+n+r}+\tfrac{(a_r-b_r)}{4}\sigma^y_j\sigma^z_{j+1}\cdots\sigma^z_{j+n+r-1}\sigma^y_{j+n+r}\Big]\\
&-\hat{\mathcal{N}}\sum_{j=L-n-r+1}^{L}\Big[\tfrac{(a_r+b_r)}{4}\sigma^x_j\sigma^z_{j+1}\cdots\sigma^z_{j+n+r-1}\sigma^x_{j+n+r}+\tfrac{(a_r-b_r)}{4}\sigma^y_j\sigma^z_{j+1}\cdots\sigma^z_{j+n+r-1}\sigma^y_{j+n+r}\Big]\Bigg],
\end{aligned}
\tag{C.14}
$$

for the case which $n > R$. In the case of $n \leq R$ one gets

$$
\begin{aligned}
I_n^+ = &\sum_{\substack{r=0\\ r\neq n}}^{R}\Bigg[\sum_{j=1}^{L-n-r}\Big[\tfrac{a_r+b_r}{4}\sigma_j^x\sigma_{j+1}^z\cdots\sigma_{j+n+r-1}^z\sigma_{j+n+r}^x+\tfrac{a_r-b_r}{4}\sigma_j^y\sigma_{j+1}^z\cdots\sigma_{j+n+r-1}^z\sigma_{j+n+r}^y\Big]\\
&+\sum_{j=1}^{L+n-r}\Big[\tfrac{a_r+b_r}{4}\sigma_{j+n}^x\sigma_{j+n+1}^z\cdots\sigma_{j+r-1}^z\sigma_{j+r}^x+\tfrac{a_r-b_r}{4}\sigma_{j+n}^y\sigma_{j+n+1}^z\cdots\sigma_{j+r-1}^z\sigma_{j+r}^y\Big] \qquad \text{(C.15)}\\
&-\hat{\mathcal{N}}\sum_{j=L-n-r+1}^{L}\Big[\tfrac{a_r+b_r}{4}\sigma_j^x\sigma_{j+1}^z\cdots\sigma_{j+n+r-1}^z\sigma_{j+n+r}^x+\tfrac{a_r-b_r}{4}\sigma_j^y\sigma_{j+1}^z\cdots\sigma_{j+n+r-1}^z\sigma_{j+n+r}^y\Big]\\
&-\hat{\mathcal{N}}\sum_{j=L+n-r+1}^{L}\Big[\tfrac{a_r+b_r}{4}\sigma_{j+n}^x\sigma_{j+n+1}^z\cdots\sigma_{j+r-1}^z\sigma_{j+r}^x+\tfrac{a_r-b_r}{4}\sigma_{j+n}^y\sigma_{j+n+1}^z\cdots\sigma_{j+r-1}^z\sigma_{j+r}^y\Big]\Bigg]\\
&+\frac{a_n}{2}\sum_{j\in\Lambda}\sigma_j^z.
\end{aligned}
$$

There is also the possibility to write the spin form of our quantities of interest in a way that operator $\hat{\mathcal{N}}$ does not appear explicitly. As it can be seen, whenever a product of two fermionic operators at sites i and j is written in the Pauli spin operators, there is a string of σ^z between these two sites. As in equations (C.15) and (C.14), we placed the string of spin-z operator in the smallest path between our lattice sites. However, In the boundary terms, this smallest path is passing through the boundary. Therefore, we face terms like $\cdots\sigma_L^z\sigma_1^z\cdots$ accompanied with operator $\hat{\mathcal{N}}$. If before the JW-transformation, we rearrange our fermionic operators $c_i^{(\dagger)}$ and $c_j^{(\dagger)}$ in a way that the operator with smaller index comes on the left of the operator with a bigger index. In particular, one can write:

$$
c_{L-n}^\dagger c_m + c_m^\dagger c_{L-n} \longrightarrow (\sigma_m^x\sigma_{L-n}^x+\sigma_m^y\sigma_{L-n}^y)\prod_{j=m+1}^{L-n-1}\sigma_j^z, \qquad \text{(C.16)}
$$

where $n, m < \frac{L}{2}$. This way of writing the integrals of motion eliminates the operator $\hat{\mathcal{N}}$ and both of these methods are equivalent. For example for I_n^+ with $n > R$ can be written as

$$
I_n^+ = \sum_{r=0}^{R}\sum_{1\leq i<j\leq L}\Big[(\tfrac{(a_r+b_r)}{4}\sigma_i^x\sigma_j^x+\tfrac{(a_r-b_r)}{4}\sigma_i^y\sigma_j^y)\prod_{k=j+1}^{l-1}\sigma_k^z\Big], \qquad \text{(C.17)}
$$

which $j = i \pm r + n$, and since $n > r$ for all r then $j > i$ for all r.

Entanglement entropy in the free fermions: the method of correlations

For the free fermions one can use the matrix of correlations to calculate the entanglement entropy for relatively large sizes. In this subsection we provide the well-known exact formulas that can be found in the reviews[69, 91]. The entanglement entropy for the eigenstates of the free fermions (XX-chain) can be found using the following formula:

$$
S_{vN} = -\sum_j \lambda_j \ln\lambda_j + (1-\lambda_j)\ln(1-\lambda_j), \qquad \text{(C.18)}
$$

where λ_j's are the eigenvalues of the correlation matrix $\mathbf{C}_A$ restricted to the subsystem A with the elements $C_{ij} = \langle c_i^\dagger c_j \rangle$.

Structure of degeneracies and average entanglement over excited states of the XX-chain

In this appendix, we tend to present a detailed study of various averagings of entanglement entropy for a periodic free fermion system in excited states. By excited states, we mean eigenstates of Hamiltonian produced by the action of $\eta_k^\dagger$ on the vacuum state of the XX-chain; Among these states, there are sets of degenerate states. In [102], the authors calculated the entanglement entropy for all the states produced as explained above, and then they took the average of all the entropies calculated without counting for degenerate states. Here, we revisit the work of [102] by taking into account the degeneracies. First, we identify the degenerate states and then preform various averagings on the entanglement entropies.

Degenerate Energy States: The XX-chain can be solved exactly by diagonalizing the Hamiltonian using the Fourier transformation, as written in the main text. Each excited state can be produced by acting on the vacuum with a set of creation operators with different modes. Each mode η_k has energy

$$|f(k)|; \qquad k = 1, 2, \cdots, L, \tag{C.19}$$

where L is the size of the system. For instance, states $|\psi^m\rangle$ and $|\psi^n\rangle$ can be degenerate ($E^m = E^n$) but they are made of different combinations of $\eta^\dagger$'s.

$$\begin{aligned} |\psi^m\rangle &= \eta_{m_1}^\dagger \eta_{m_2}^\dagger \eta_{m_3}^\dagger \cdots |0\rangle, \\ |\psi^n\rangle &= \eta_{n_1}^\dagger \eta_{n_2}^\dagger \eta_{n_3}^\dagger \cdots |0\rangle, \end{aligned}$$

in a way that

$$\{k_{m_1}, k_{m_2}, k_{m_3}, \cdots\} \neq \{k_{n_1}, k_{n_2}, k_{n_3}, \cdots\}.$$

For instance in XX model, the energy of the modes with $k = l$ and $k = L - l$ is the same, therefore the degeneracy in the eigenstates is expected. To unravel these groups of degenerate eigenstates as accurate as possible (machine precision), we first calculated the minimum energy gap (ΔE_{min}) of the spectrum. Since in these types of Hamiltonians the energy levels are not equally spaced, the ΔE_{min} helps us to have an idea for the required precision value to decide whether two energies are equal or not. Not surprisingly, as shown in the inset of the figure 12, this gap decreases exponentially with the size of the system which makes the decision that two states are degenerate or not more difficult by increasing the size of the system. After finding all the degeneracies, we sum over all

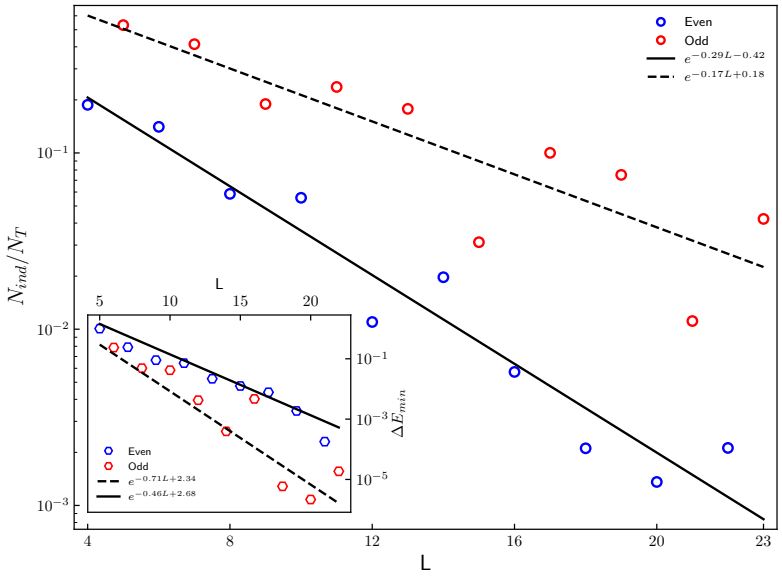


Figure 12 – In this figure, the ratio of independent energies to total number of energies is plotted versus the system size. $\frac{N_{ind}}{N_T}$ decreases exponentially with size of the system. (Inset) Plot of ΔE_{min} versus the size of the system. This quantity gives us a measure to set a precision for finding the unequal energy levels of the spectrum. Note that for L even we have degeneracy even in the level of the energy modes which is the main reason for stronger decay of $\frac{N_{ind}}{N_T}$ with respect to the L odd case.

the non-degenerate states and call the number N_{ind}. This number which we loosely call the number of independent states is exponentially smaller than the dimension of the Hilbert space. In other words, as shown in the figure 12, the ratio $\frac{N_{ind}}{N_T}$ decays exponentially with the size of the system L. This indicates the presence of an enormous amount of degeneracies in the spectrum of the XX-chain.

— D —

Appendix of Chapter 7

Correlations for excited quasiparticle eigenstates

In section 7.3, we introduced the correlation functions and the method to produce these matrices for the ground state. In this part, we are going to present the method to calculate the correlations for excited quasiparticles (7.27) using the unitary transformation $\mathbf{U}$ which diagonalize the Hamiltonian.

The quasiparticle excited state such as $|\psi\rangle$ is defined by

$$|\psi\rangle = |k_1, k_2, \cdots, k_N\rangle = \prod_{k_j \in \mathbb{E}} \eta^\dagger_{k_j} |0\rangle_\eta \tag{D.1}$$

where set $\mathbb{E}$ could be any subset of modes. For this state, we start by calculating the $\langle\psi| c^\dagger_i c_j |\psi\rangle$ and $\langle\psi| c^\dagger_i c^\dagger_j |\psi\rangle$

$$\langle c^\dagger_i c_j\rangle_\psi = \langle 0| \prod_{k_j \in \mathbb{E}} \eta_{k_j} \sum_{k,l} (h^*_{li}\eta_l + g_{ki}\eta^\dagger_k) \sum_{n,m} (g^*_{mj}\eta_m + h_{nj}\eta^\dagger_n) \prod_{k_j \in \mathbb{E}} \eta^\dagger_{k_j} |0\rangle\,, \tag{D.2}$$

$$\langle c^\dagger_i c^\dagger_j\rangle_\psi = \langle 0| \prod_{k_j \in \mathbb{E}} \eta_{k_j} \sum_{k,l} (h^*_{li}\eta_l + g_{ki}\eta^\dagger_k) \sum_{n,m} (h^*_{mj}\eta_m + g_{nj}\eta^\dagger_n) \prod_{k_j \in \mathbb{E}} \eta^\dagger_{k_j} |0\rangle\,. \tag{D.3}$$

Using the Wick theorem we can simplify these expressions to get:

$$\begin{aligned} \langle c^\dagger_i c_j\rangle_\psi &= (\mathbf{h}^\dagger.\mathbf{h})_{i,j} + \sum_{k_j \in \mathbb{E}} (g_{k_j,i} g^*_{k_j,j} - h^*_{k_j,i} h_{k_j,j}), \\ \langle c^\dagger_i c^\dagger_j\rangle_\psi &= (\mathbf{h}^\dagger.\mathbf{g})_{i,j} + \sum_{k_j \in \mathbb{E}} (g_{k_j,i} h^*_{k_j,j} - h^*_{k_j,i} g_{k_j,j}). \end{aligned} \tag{D.4}$$

Therefore, using the definitions (7.51), we can write the $\mathbf{K}$, $\bar{\mathbf{K}}$ and $\mathbf{G}$ for the state $|\psi\rangle$ in a short version as

$$\mathbf{K}^\psi_{ij} = (\mathbf{h}^\dagger + \mathbf{g}^\dagger).(\mathbf{h} + \mathbf{g})_{ij} - 2i\Im\Big[\sum_{k_j \in \mathbb{E}} (h^*_{k_j,i} + g^*_{k_j,i})(g_{k_j,j} + h_{k_j,j})\Big], \tag{D.5}$$

$$\bar{\mathbf{K}}^\psi_{ij} = (\mathbf{h}^\dagger - \mathbf{g}^\dagger).(\mathbf{h} - \mathbf{g})_{ij} - 2i\Im\Big[\sum_{k_j \in \mathbb{E}} (h^*_{k_j,i} - g^*_{k_j,i})(h_{k_j,j} - g_{k_j,j})\Big], \tag{D.6}$$

$$\mathbf{G}^\psi_{ij} = (\mathbf{h}^\dagger - \mathbf{g}^\dagger).(\mathbf{h} + \mathbf{g})_{ij} + 2\Re\Big[\sum_{k_j \in \mathbb{E}} (g^*_{k_j,i} - h^*_{k_j,i})(h_{k_j,j} + g_{k_j,j})\Big]. \tag{D.7}$$

The prior expressions are useful for the study of entanglement in excited quasiparticle states. One can use the $\mathbf{\Gamma}^\psi$ to calculate the RDM for a given subsystem A using the relation

$$\rho^\psi_A(\boldsymbol{\gamma}, \bar{\boldsymbol{\gamma}}) = [\det \frac{\mathbf{I} - \mathbf{\Gamma}^\psi_A}{2}]^{\frac{1}{2}} e^{\frac{1}{4}\begin{pmatrix}\boldsymbol{\gamma} & \bar{\boldsymbol{\gamma}}\end{pmatrix} \ln \frac{\mathbf{I}+\mathbf{\Gamma}^\psi_A}{\mathbf{I}-\mathbf{\Gamma}^\psi_A} \begin{pmatrix}\boldsymbol{\gamma} \\ \bar{\boldsymbol{\gamma}}\end{pmatrix}}, \tag{D.8}$$

where γ and $\bar{\gamma}$ are the Majorana fermions defined in section 7.3. Equivalently, it is possible to use the preceding correlations to find the $\mathbf{R}^{\psi}$ matrix (as in (7.28)), $\mathbf{R}^{\psi} = \mathbf{F}^{\psi *}(\mathbf{I}-\mathbf{C}^{\psi})^{-1}$, which could lead to finding the RDM.

For excited states created from ZME state, we can do the same calculations. These quasiparticle excited state are created as:

$$\left|\phi_{\emptyset}\right\rangle = |n_1, n_2, \cdots, n_N\rangle = \prod_{n_j \in \mathbb{E}} \eta^{\dagger}_{n_j} |\emptyset\rangle \,, \tag{D.9}$$

where $n_j \neq 0$. Having the correlation matrices for the above states allows us to study the excited state entanglement for these states likewise. To write such matrices, we can use the result of section 7.3.2. Correlations for the family of ZME excited states are demonstrated in 166. The matrices $\mathbf{K}^{\phi_{\emptyset}}$ and $\bar{\mathbf{K}}^{\phi_{\emptyset}}$ have the same form as (D.5) and (D.6), therefore, we have not included their forms.

As it was explained in subsection 7.2.6, one could divide the Hilbert space of Hamiltonian (7.5) into four different towers which one of the these towers or sectors corresponds to the eigenstates of boundary magnetic field Hamiltonian (7.1). We devote this part to find the correlation functions for states in a given tower, given the ground state for the tower (sector), can be found with $|G_{\pm}\rangle$. The base of calculation is similar to the above cases, therefore here we only hand out the final result. For start, an excited state in one of the sectors has the form

$$\left|\chi_{\pm}\right\rangle = \prod_{m_j \in \mathbb{E}} \eta^{\dagger}_{m_j} \left|G_{\pm}\right\rangle . \tag{D.10}$$

In the preceding expression, set $\mathbb{E}$ contains excited modes acting on $\left|G_{\pm}\right\rangle$ and $0 \notin \mathbb{E}$. For a general case of $\mathbb{E}$ we can write the correlations as in page 167. Similar to the ZME and the $|G_{\pm}\rangle$ case, the matrices $\mathbf{K}^{\chi_{\pm}}$ and $\bar{\mathbf{K}}^{\chi_{\pm}}$ have the same form as $\mathbf{K}^{\psi}$ and $\bar{\mathbf{K}}^{\psi}$ in (D.5) and (D.6).

$$
\mathbf{C}^{\phi_\emptyset} = \begin{pmatrix} \frac{1}{2} & C^{\emptyset}_{0,j} + \sum_{n\in\mathbb{E}} (g_{n,0} g^*_{n,j} + g^*_{n,0} h_{n,j}) & C^{\emptyset}_{0,L+1} + \sum_{n\in\mathbb{E}} (g_{n,0} g^*_{n,L+1} + g^*_{n,0} g_{n,L+1}) \\ C^{\emptyset}_{i,0} + \sum_{n\in\mathbb{E}} (g_{n,i} g^*_{n,0} + h^*_{n,i} g_{n,0}) & C^{\emptyset}_{i,j} + \sum_{n\in\mathbb{E}} (g_{n,i} g^*_{n,j} - h^*_{n,i} h_{n,j}) & C^{\emptyset}_{i,L+1} + \sum_{n\in\mathbb{E}} (g_{n,i} g^*_{n,L+1} - h^*_{n,i} g_{n,L+1}) \\ C^{\emptyset}_{L+1,0} + \sum_{n\in\mathbb{E}} (g_{n,L+1} g^*_{n,0} + g^*_{n,L+1} g_{n,0}) & C^{\emptyset}_{L+1,j} + \sum_{n\in\mathbb{E}} (g_{n,L+1} g^*_{n,j} - g^*_{n,L+1} h_{n,j}) & \frac{1}{2} \end{pmatrix}, \tag{D.11}
$$

$$
\mathbf{F}^{\phi_\emptyset} = \begin{pmatrix} 0 & F^{\emptyset}_{0,j} + \sum_{n\in\mathbb{E}} (g_{n,0} h^*_{n,j} + g^*_{n,0} g_{n,j}) & F^{\emptyset}_{0,L+1} + \sum_{n\in\mathbb{E}} (g_{n,0} g^*_{n,L+1} + g^*_{n,0} g_{n,L+1}) \\ F^{\emptyset}_{i,0} - \sum_{n\in\mathbb{E}} (g_{n,i} g^*_{n,0} + h^*_{n,i} g_{n,0}) & F^{\pm}_{i,j} + \sum_{n\in\mathbb{E}} (g_{n,i} h^*_{n,j} - h^*_{n,i} g_{n,j}) & F^{\emptyset}_{i,L+1} + \sum_{n\in\mathbb{E}} (g_{n,i} g^*_{n,L+1} - g^*_{n,i} g_{n,L+1}) \\ F^{\emptyset}_{L+1,0} - \sum_{n\in\mathbb{E}} (g_{n,L+1} g^*_{n,0} + g^*_{n,L+1} g_{n,0}) & F^{\emptyset}_{L+1,j} + \sum_{n\in\mathbb{E}} (g_{n,L+1} h^*_{n,j} - g^*_{n,L+1} g_{n,j}) & 0 \end{pmatrix}, \tag{D.12}
$$

$$
\mathbf{G}^{\phi_\emptyset} = \begin{pmatrix} 0 & G^{\emptyset}_{0,j} + 4\Re\big[\sum_{n\in\mathbb{E}} g^*_{n,0}(h_{n,j} + g_{n,j})\big] & G^{\emptyset}_{0,L+1} + 8\Re\big[\sum_{n\in\mathbb{E}} g^*_{n,0} g_{n,L+1}\big] \\ 0 & G^{\emptyset}_{i,j} + 2\Re\big[\sum_{n\in\mathbb{E}} (g^*_{n,0} - h^*_{n,0})(h_{n,j} + g_{n,j})\big] & G^{\emptyset}_{i,L+1} + 4\Re[\sum_{n\in\mathbb{E}} (g^*_{n,i} - h^*_{n,i}) g_{n,L+1}] \\ 1 & 0 & 0 \end{pmatrix}. \tag{D.13}
$$

$$\mathbf{C}^{\chi_\pm}=\begin{pmatrix} \frac{1}{2} & C^{\pm}_{0,j}+\sum_{m\in\mathbb{E}}\left(g_{m,0}g^*_{m,j}+g^*_{m,0}h_{m,j}\right) & C^{\pm}_{0,L+1}+\sum_{m\in\mathbb{E}}\left(g_{m,0}g^*_{m,L+1}+g^*_{m,0}g_{m,L+1}\right)\\ C^{\pm}_{i,0}+\sum_{m\in\mathbb{E}}\left(g_{m,i}g^*_{m,0}+h^*_{m,i}g_{m,0}\right) & C^{\pm}_{i,j}+\sum_{m\in\mathbb{E}}\left(g_{m,i}g^*_{m,j}-h^*_{m,i}h_{m,j}\right) & C^{\pm}_{i,L+1}+\sum_{m\in\mathbb{E}}\left(g_{m,i}g^*_{m,L+1}-h^*_{m,i}g_{m,L+1}\right)\\ C^{\pm}_{L+1,0}+\sum_{m\in\mathbb{E}}\left(g_{m,L+1}g^*_{m,0}+g^*_{m,L+1}g_{m,0}\right) & C^{\pm}_{L+1,j}+\sum_{m\in\mathbb{E}}\left(g_{m,L+1}g^*_{m,j}-g^*_{m,L+1}h_{m,j}\right) & \frac{1}{2}\end{pmatrix}, \tag{D.14}$$

$$\mathbf{F}^{\chi_\pm}=\begin{pmatrix} 0 & F^{\pm}_{0,j}+\sum_{m\in\mathbb{E}}\left(g_{m,0}h^*_{m,j}+g^*_{m,0}g_{m,j}\right) & F^{\pm}_{0,L+1}+\sum_{m\in\mathbb{E}}\left(g_{m,0}g^*_{m,L+1}+g^*_{m,0}g_{m,L+1}\right)\\ F^{\pm}_{i,0}-\sum_{m\in\mathbb{E}}\left(g_{m,i}g^*_{m,0}+h^*_{m,i}g_{m,0}\right) & F^{\pm}_{i,j}+\sum_{m\in\mathbb{E}}\left(g_{m,i}h^*_{m,j}-h^*_{m,i}g_{m,j}\right) & F^{\pm}_{i,L+1}+\sum_{m\in\mathbb{E}}\left(g_{m,i}g^*_{m,L+1}-g^*_{m,i}g_{m,L+1}\right)\\ F^{\pm}_{L+1,0}-\sum_{m\in\mathbb{E}}\left(g_{m,L+1}g^*_{m,0}+g^*_{m,L+1}g_{m,0}\right) & F^{\pm}_{L+1,j}+\sum_{m\in\mathbb{E}}\left(g_{m,L+1}h^*_{m,j}-g^*_{m,L+1}g_{m,j}\right) & 0\end{pmatrix}, \tag{D.15}$$

$$\mathbf{G}^{\chi_\pm}=\begin{pmatrix} 0 & G^{\pm}_{0,j}+4\Re\Big[\sum_{m\in\mathbb{E}}g^*_{m,0}(h_{m,j}+g_{m,j})\Big] & G^{\pm}_{0,L+1}+8\Re\Big[\sum_{m\in\mathbb{E}}g^*_{m,0}g_{m,L+1}\Big]\\ 0\,G^{\pm}_{i,j}+2\Re\Big[\sum_{m\in\mathbb{E}}(g^*_{m,0}-h^*_{m,0})(h_{m,j}+g_{m,j})\Big] & G^{\pm}_{i,L+1}+4\Re\Big[\sum_{m\in\mathbb{E}}(g^*_{m,i}-h^*_{m,i})g_{m,L+1}\Big] & \\ 0 & 0 & 0\end{pmatrix}. \tag{D.16}$$

Reduced density matrix calculations

In this appendix, we are presenting the calculations of (7.74) in details. Starting from (7.70), we can write

$$\begin{aligned}\rho_{\mathbf{1}}^{\beta}(\boldsymbol{\xi},\boldsymbol{\xi}') =& \int \prod_{l\in\mathbf{2}} \mathrm{d}\bar{\xi}_l \mathrm{d}\xi_l \; e^{-\sum\limits_{n\in\mathbf{2}} \bar{\xi}_n \xi_n} \langle \xi_1, \cdots, \xi_k, -\xi_{k+1}, \cdots, -\xi_L | \, \rho^{\beta} \, | \xi_1', \cdots, \xi_k', \xi_{k+1}, \cdots, \xi_L \rangle \\ =& |C^{\beta}|^2 e^{\frac{1}{2}(\mathbf{R}_{11})_{ij}\bar{\xi}_i\bar{\xi}_j - \frac{1}{2}(\mathbf{R}_{11}^*)_{ji}\xi_j'\xi_i'} \int \prod_{l\in\mathbf{2}} \mathrm{d}\bar{\xi}_l \mathrm{d}\xi_l \; e^{-\bar{\xi}_n\xi_n} \mathcal{F}(\{\xi_n\},\{\xi_i'\},\{\bar{\xi}_j\},\{\bar{\xi}_m\}) \\ & \times \Big[e^{-\frac{1}{2}(\mathbf{R}_{12})_{in}\bar{\xi}_i\bar{\xi}_n - \frac{1}{2}(\mathbf{R}_{21})_{ni}\bar{\xi}_n\bar{\xi}_i} e^{\frac{1}{2}(\mathbf{R}_{22})_{mn}\bar{\xi}_m\bar{\xi}_n} e^{-\frac{1}{2}(\mathbf{R}_{22}^*)_{nm}\xi_n\xi_m + \frac{1}{2}(\mathbf{R}_{12}^*)_{jm}\xi_j'\xi_m + \frac{1}{2}(\mathbf{R}_{21}^*)_{mj}\xi_m\xi_j'} \Big], \end{aligned} \tag{D.17}$$

where in the above Einstein summation convention is used. To clarify the notation above, the indices i, j belong to subsystem $\mathbf{1}$ and indices n, m to subsystem $\mathbf{2}$. Eventually, the function $\mathcal{F}$ is given by

$$\begin{aligned}\mathcal{F}(\{\xi_n\},\{\xi_i'\},\{\bar{\xi}_j\},\{\bar{\xi}_m\}) =& \, 1 + \beta(\mathfrak{M}_1)_{0j}\bar{\xi}_j - \beta(\mathfrak{M}_2)_{0m}\bar{\xi}_m + \beta^*(\mathfrak{M}_1^*)_{0i}\xi_i' \\ & + \beta^*(\mathfrak{M}_2^*)_{0n}\xi_n + |\beta|^2(\mathfrak{M}_1)_{0j}(\mathfrak{M}_1^*)_{0i}\bar{\xi}_j\xi_i' + |\beta|^2(\mathfrak{M}_1)_{0j}(\mathfrak{M}_2^*)_{0n}\bar{\xi}_j\xi_n \\ & - |\beta|^2(\mathfrak{M}_2)_{0m}(\mathfrak{M}_1^*)_{0i}\bar{\xi}_m\xi_i' - |\beta|^2(\mathfrak{M}_2)_{0m}(\mathfrak{M}_2^*)_{0n}\bar{\xi}_m\xi_n. \end{aligned} \tag{D.18}$$

In (D.17) we have divided $\mathbf{R}$ into four submatrices $\mathbf{R_{11}}$, $\mathbf{R_{12}}$, $\mathbf{R_{21}} = -\mathbf{R_{12}}^T$ and $\mathbf{R_{22}}$, according to the part we are tracing out (or not). Although these submatrices do not need to have same size, $\mathbf{R_{11}}$ and $\mathbf{R_{22}}$ should be square matrices. We write the (D.17) in the compact form:

$$\rho_{\mathbf{1}}(\boldsymbol{\xi},\boldsymbol{\xi}') = |C^{\beta}|^2 e^{\frac{1}{2}\begin{pmatrix}\bar{\boldsymbol{\xi}} & \boldsymbol{\xi}'\end{pmatrix}\begin{pmatrix}\mathbf{R}_{11} & 0 \\ 0 & -\mathbf{R}_{11}^*\end{pmatrix}\begin{pmatrix}\bar{\boldsymbol{\xi}} \\ \boldsymbol{\xi}'\end{pmatrix}} \int \mathbf{D}\boldsymbol{\eta} \mathcal{F}(\boldsymbol{\xi}_i', \bar{\boldsymbol{\xi}}_j, \boldsymbol{\eta}) e^{\frac{1}{2}\boldsymbol{\eta}^T\boldsymbol{\mathcal{A}}\boldsymbol{\eta} + \boldsymbol{\lambda}^T\boldsymbol{\eta}}. \tag{D.19}$$

where $\mathbf{D}\boldsymbol{\eta} = \mathrm{d}\bar{\xi}\mathrm{d}\xi$ and

$$\boldsymbol{\eta}^T = \begin{pmatrix}\bar{\boldsymbol{\xi}} & \boldsymbol{\xi}\end{pmatrix}, \qquad \boldsymbol{\lambda}^T = \begin{pmatrix}-\bar{\boldsymbol{\xi}}\mathbf{R}_{12} & -\boldsymbol{\xi}'\mathbf{R}_{12}^*\end{pmatrix}, \tag{D.20}$$

$$\boldsymbol{\mathcal{A}} = \begin{pmatrix}\mathbf{R}_{22} & -\mathbf{I} \\ \mathbf{I} & -\mathbf{R}_{22}^*\end{pmatrix}. \tag{D.21}$$

It is much easier to solve the integration in (D.19) with this new variables. In the expression of $\mathcal{F}$, the first, second, forth and sixth terms do not depend on the variables of integration. Therefore, for those terms we can write:

$$\rho_{\mathbf{1}}^{\beta}(1^{\mathrm{st}}, 2^{\mathrm{nd}}, 4^{\mathrm{th}}, 6^{\mathrm{th}}, \boldsymbol{\xi}, \boldsymbol{\xi}') = |C^{\beta}|(\det\boldsymbol{\mathcal{A}})^{\frac{1}{2}}\Big(1 + \beta\mathfrak{M}_1\bar{\boldsymbol{\xi}}\Big)\Big(1 + \beta^*\mathfrak{M}_1^*\boldsymbol{\xi}'\Big) e^{\frac{1}{2}\begin{pmatrix}\bar{\xi} & \xi'\end{pmatrix}\boldsymbol{\Omega}\begin{pmatrix}\bar{\xi} \\ \xi'\end{pmatrix}}, \tag{D.22}$$

where

$$\mathbf{\Omega}=\begin{pmatrix}\mathbf{R}_{11} & 0\\ 0 & -\mathbf{R}_{11}{}^{*}\end{pmatrix}+\begin{pmatrix}\mathbf{R}_{12} & 0\\ 0 & \mathbf{R}_{12}{}^{*}\end{pmatrix}\boldsymbol{\mathcal{A}}^{-1}\begin{pmatrix}\mathbf{R}_{12}{}^{T} & 0\\ 0 & \mathbf{R}_{12}{}^{\dagger}\end{pmatrix}. \tag{D.23}$$

For the terms with linear Grassmann variables in the integration we first substitute $\boldsymbol{\eta}\rightarrow\boldsymbol{\eta}+\boldsymbol{\mathcal{A}}^{-1}\boldsymbol{\lambda}$ in (D.19). Using the Berezin integration techniques in presented in [58], we are left with

$$\rho_{\mathbf{1}}^{\beta}(3^{\text{rd}},5^{\text{th}},7^{\text{th}},8^{\text{th}},\boldsymbol{\xi},\boldsymbol{\xi}')=|C^{\beta}|(\det\Big[\boldsymbol{\mathcal{A}}\Big])^{\frac{1}{2}}(\det\Big[\boldsymbol{\mathcal{W}}\Big])^{\frac{1}{2}}F(\bar{\boldsymbol{\xi}}_{\mathbf{1}},\boldsymbol{\xi}'_{\mathbf{1}})e^{\frac{1}{2}\begin{pmatrix}\bar{\xi} & \xi'\end{pmatrix}\mathbf{\Omega}\begin{pmatrix}\bar{\xi}\\ \xi'\end{pmatrix}}, \tag{D.24}$$

with

$$\begin{aligned}F(\bar{\boldsymbol{\xi}}_{\mathbf{1}},\boldsymbol{\xi}'_{\mathbf{1}}) &= |\beta|^{2}\text{Pf}\Big[\boldsymbol{\mathcal{W}}\Big]+\begin{pmatrix}-\beta\mathfrak{M}_{2} & 0\\ 0 & \beta^{*}\mathfrak{M}_{2}^{*}\end{pmatrix}\boldsymbol{\mathcal{A}}^{-1}\boldsymbol{\lambda}+|\beta|^{2}\mathfrak{M}_{1}\bar{\boldsymbol{\xi}}\times\begin{pmatrix}0 & 0\\ 0 & \mathfrak{M}_{2}^{*}\end{pmatrix}\boldsymbol{\mathcal{A}}^{-1}\boldsymbol{\lambda} \qquad \text{(D.25)}\\ &\quad +|\beta|^{2}\begin{pmatrix}-\mathfrak{M}_{2} & 0\\ 0 & 0\end{pmatrix}\boldsymbol{\mathcal{A}}^{-1}\boldsymbol{\lambda}\times\mathfrak{M}_{1}^{*}\boldsymbol{\xi}'+|\beta|^{2}\begin{pmatrix}-\mathfrak{M}_{2} & 0\end{pmatrix}\boldsymbol{\mathcal{A}}^{-1}\boldsymbol{\lambda}\times\begin{pmatrix}0 & \mathfrak{M}_{2}{}^{*}\end{pmatrix}\boldsymbol{\mathcal{A}}^{-1}\boldsymbol{\lambda},\\ \boldsymbol{\mathcal{W}} &= \begin{pmatrix}\mathfrak{M}_{2} & \mathbf{0}\\ \mathbf{0} & -\mathfrak{M}_{2}^{*}\end{pmatrix}\boldsymbol{\mathcal{A}}^{-T}\begin{pmatrix}\mathfrak{M}_{2}^{T} & \mathbf{0}\\ \mathbf{0} & -\mathfrak{M}_{2}^{\dagger}\end{pmatrix}. \qquad \text{(D.26)}\end{aligned}$$

Putting (D.22) and (D.24) together, after some algebraic manipulations, we get to (7.71).

We could have used another trick to solve the Berezin integrations to get RDM. This method ends up in having two exponentials in the final result. The trick is to write the linear Grassmann variable in the integration as exponentials, like:

$$(\mathfrak{M}\bar{\boldsymbol{\xi}})_{k_1}\cdots(\mathfrak{M}\bar{\boldsymbol{\xi}})_{k_N}\Big(\mathfrak{M}^{*}\boldsymbol{\xi}'\Big)_{k_1}\cdots\Big(\mathfrak{M}^{*}\boldsymbol{\xi}'\Big)_{k_N}=\int\prod_{i}\mathrm{d}\bar{\theta}_{i}\mathrm{d}\theta_{i}e^{\sum_{k_j}\theta_{k_j}(\mathfrak{M}\bar{\boldsymbol{\xi}})_{k_j}+\bar{\theta}_{k_j}(\mathfrak{M}^{*}\boldsymbol{\xi})_{k_j}}. \tag{D.27}$$

In the above relation, θ and $\bar{\theta}$ are Grassmann variables too.

If we start again from density matrix expression in coherent basis (7.69), and rewrite it as:

$$\begin{aligned}\rho^{\beta}(\boldsymbol{\xi},\boldsymbol{\xi}') =&|C^{\beta}|^{2}e^{\frac{1}{2}R_{ij}\bar{\xi}_{i}\bar{\xi}_{j}}(1+\beta\mathfrak{M}_{0k}\bar{\xi}_{k}+\beta^{*}\mathfrak{M}_{0l}^{*}\xi'_{l}+|\beta|^{2}\mathfrak{M}_{0k}\mathfrak{M}_{0l}^{*}\bar{\xi}_{k}\xi'_{l})e^{-\frac{1}{2}R_{nm}^{*}\xi'_{n}\xi'_{m}}\\ =&\rho^{\beta}(1,\boldsymbol{\xi},\boldsymbol{\xi}')+\varrho^{\beta}(2,\boldsymbol{\xi},\boldsymbol{\xi}')+\varrho^{\beta}(3,\boldsymbol{\xi},\boldsymbol{\xi}')+\rho^{\beta}(4,\boldsymbol{\xi},\boldsymbol{\xi}'),\end{aligned} \tag{D.28}$$

where the $\rho^{\beta}(1,\boldsymbol{\xi},\boldsymbol{\xi}')$ and $\rho^{\beta}(4,\boldsymbol{\xi},\boldsymbol{\xi}')$ are the density matrices corresponding to the vacuum-vacuum state and excited-excited state, and the $\varrho^{\beta}(2,\boldsymbol{\xi},\boldsymbol{\xi}')$ and $\varrho^{\beta}(3,\boldsymbol{\xi},\boldsymbol{\xi}')$ are density cross

terms corresponding to the vacuum-excited (and exited-vacuum) state terms. We are going to partial trace each term separately and then put the results together afterwards. For the first term in (D.28), we have:

$$\rho_{\mathbf{1}}^{\beta}(1,\boldsymbol{\xi},\boldsymbol{\xi}') = \frac{\mathcal{C}^{\beta}}{|\beta|^2} e^{\frac{1}{2}\begin{pmatrix}\bar{\xi} & \xi'\end{pmatrix}\boldsymbol{\Omega}^{\beta}\begin{pmatrix}\bar{\xi}\\ \xi'\end{pmatrix}}, \tag{D.29}$$

where again

$$\mathcal{C}^{\beta} = \frac{|\beta|^2\sqrt{\det\left[\mathbf{I}+\mathbf{R}_{22}{}^{\dagger}\mathbf{R}_{22}\right]}}{(1+|\beta|^2)\sqrt{\det\left[\mathbf{I}+\mathbf{R}^{\dagger}\mathbf{R}\right]}}, \qquad \boldsymbol{\mathcal{A}} = \begin{pmatrix}\mathbf{R}_{22} & -\mathbf{I}\\ \mathbf{I} & -\mathbf{R}_{22}^{*}\end{pmatrix}, \tag{D.30a}$$

$$\boldsymbol{\Omega} = \begin{pmatrix}\mathbf{R}_{11} & 0\\ 0 & -\mathbf{R}_{11}{}^{*}\end{pmatrix} + \begin{pmatrix}\mathbf{R}_{12} & 0\\ 0 & \mathbf{R}_{12}{}^{*}\end{pmatrix}\boldsymbol{\mathcal{A}}^{-1}\begin{pmatrix}\mathbf{R}_{12}{}^{T} & 0\\ 0 & \mathbf{R}_{12}{}^{\dagger}\end{pmatrix}. \tag{D.30b}$$

For the last term in (D.28), we can write:

$$\rho^{\beta}(4,\boldsymbol{\xi},\boldsymbol{\xi}') = |C^{\beta}\beta|^2\int \mathrm{d}\bar{\theta}\mathrm{d}\theta e^{\theta(\mathfrak{M}\bar{\xi})+\bar{\theta}(\mathfrak{M}^{*}\boldsymbol{\xi}')}e^{\frac{1}{2}R_{ij}\bar{\xi}_i\bar{\xi}_j}e^{-\frac{1}{2}R_{ij}^{*}\xi_i'\xi_j'}. \tag{D.31}$$

For the reduced density matrix we get

$$\begin{aligned}\rho_{\mathbf{1}}^{\beta}(4,\boldsymbol{\xi},\boldsymbol{\xi}') =& |C^{\beta}\beta|^2\int \mathrm{d}\bar{\theta}\mathrm{d}\theta e^{\frac{1}{2}(\mathbf{R}_{11})_{ij}\bar{\xi}_i\bar{\xi}_j-\frac{1}{2}(\mathbf{R}_{11}^{*})_{ji}\xi_j'\xi_i'}e^{\theta(\mathfrak{M}_{\mathbf{1}}\cdot\bar{\boldsymbol{\xi}})+\bar{\theta}(\mathfrak{M}_{\mathbf{1}}^{*}\cdot\boldsymbol{\xi}')}\int\prod_{l=k+1}^{L+1}\mathrm{d}\bar{\xi}_l\mathrm{d}\xi_l\, e^{-\bar{\xi}_l\xi_l}\\ &\times e^{-\theta(\mathfrak{M}_{\mathbf{2}}\bar{\boldsymbol{\xi}})+\bar{\theta}(\mathfrak{M}_{\mathbf{2}}^{*}\boldsymbol{\xi})}\left[e^{-(\mathbf{R}_{12})_{in}\bar{\xi}_i\bar{\xi}_n+\frac{1}{2}(\mathbf{R}_{22})_{mn}\bar{\xi}_m\bar{\xi}_n}e^{-\frac{1}{2}(\mathbf{R}_{22}^{*})_{nm}\xi_n\xi_m+(\mathbf{R}_{12}^{*})_{jm}\xi_j'\xi_m}\right]\end{aligned} \tag{D.32}$$

We denote the terms on the left of second integral as $\mathcal{F}(\bar{\boldsymbol{\xi}},\boldsymbol{\xi},\theta,\bar{\theta})$. If we introduce new Grassmann variables $\boldsymbol{\eta}^T = \begin{pmatrix}\bar{\boldsymbol{\xi}} & \boldsymbol{\xi}\end{pmatrix}$ and $\boldsymbol{\lambda}^T = \begin{pmatrix}-\bar{\boldsymbol{\xi}}\mathbf{R}_{12}-\theta(\mathfrak{M})_0 & -\boldsymbol{\xi}'\mathbf{R}_{12}^{*}+\bar{\theta}(\mathfrak{M}^{*})_0\end{pmatrix}$, then we can write the integral as

$$\rho_{\mathbf{1}}^{\beta}(4,\boldsymbol{\xi},\boldsymbol{\xi}') = \int \mathrm{d}\bar{\theta}\mathrm{d}\theta\mathcal{F}(\bar{\boldsymbol{\xi}},\boldsymbol{\xi}',\theta,\bar{\theta})\int \mathbf{D}\boldsymbol{\eta}\, e^{\frac{1}{2}\boldsymbol{\eta}^T\boldsymbol{\mathcal{A}}\boldsymbol{\eta}+\boldsymbol{\lambda}^T\boldsymbol{\eta}} \tag{D.33}$$

where $\boldsymbol{\mathcal{A}}$ has been defined previously. Solving the first integral we get:

$$\rho_{\mathbf{1}}^{\beta}(4,\boldsymbol{\xi},\boldsymbol{\xi}') = \mathcal{C}^{\beta}e^{\frac{1}{2}\begin{pmatrix}\bar{\xi} & \xi'\end{pmatrix}\boldsymbol{\Omega}\begin{pmatrix}\bar{\xi}\\ \xi'\end{pmatrix}}\int \mathbf{D}\boldsymbol{\Theta}e^{\frac{1}{2}\boldsymbol{\Theta}^T\boldsymbol{\omega}\boldsymbol{\Theta}+\boldsymbol{\eta}'^T\boldsymbol{\mathcal{J}}\boldsymbol{\Theta}} \tag{D.34}$$

where $\mathbf{\Theta}^T = \begin{pmatrix} \bar{\theta} & \theta \end{pmatrix}$, $\mathbf{D\Theta} = \mathrm{d}\bar{\theta}\mathrm{d}\theta$, $\boldsymbol{\eta'}^T = \begin{pmatrix} \bar{\boldsymbol{\xi}} & \boldsymbol{\xi}' \end{pmatrix}$, and $\mathbf{\Omega}$ and $\mathcal{C}^\beta$ are given by (7.72b) and (7.72a) respectively. Finally, if we take the last integral in the equation (D.34), we get

$$\rho_{\mathbf{1}}^{\beta}(4, \boldsymbol{\xi}, \boldsymbol{\xi'}) = \mathcal{C}^\beta \mathrm{Pf}[\boldsymbol{\omega}] e^{\frac{1}{2}\begin{pmatrix} \bar{\xi} & \xi' \end{pmatrix} \mathbf{\Omega}' \begin{pmatrix} \bar{\xi} \\ \xi' \end{pmatrix}} \tag{D.35}$$

where

$$\mathbf{\Omega}' = \mathbf{\Omega} + \boldsymbol{\mathcal{J}} \boldsymbol{\omega}^{-1} \boldsymbol{\mathcal{J}}^T \tag{D.36a}$$

$$\boldsymbol{\omega} = \begin{pmatrix} 0 & (\mathfrak{M}^*_{\mathbf{2}})_0 \\ -(\mathfrak{M}_2)_0 & 0 \end{pmatrix} \boldsymbol{\mathcal{A}}^{-1} \begin{pmatrix} 0 & -(\mathfrak{M}_{\mathbf{2}})_0^T \\ (\mathfrak{M}_2)_0^\dagger & 0 \end{pmatrix}, \tag{D.36b}$$

$$\boldsymbol{\mathcal{J}} = \begin{pmatrix} -\mathbf{R}_{12} & \mathbf{0} \\ \mathbf{0} & -\mathbf{R}_{12}{}^* \end{pmatrix} \boldsymbol{\mathcal{A}}^{-1} \begin{pmatrix} \mathbf{0} & \mathfrak{M}^*_2 \\ -\mathfrak{M}_2 & \mathbf{0} \end{pmatrix} - \begin{pmatrix} \mathbf{0} & \mathfrak{M}^*_1 \\ \mathfrak{M}_1 & \mathbf{0} \end{pmatrix}. \tag{D.36c}$$

To do the same calculation for cross term $\varrho^\beta(2, \boldsymbol{\xi}, \boldsymbol{\xi'})$ in equation (D.28), we have

$$\varrho^\beta(2, \boldsymbol{\xi}, \boldsymbol{\xi'}) = |C^\beta|^2 \beta\, \mathfrak{M}_{0l} \bar{\xi}_l e^{\frac{1}{2} R_{ij} \bar{\xi}_i \bar{\xi}_j - \frac{1}{2} R^*_{ij} \xi'_i \xi'_j} \tag{D.37}$$

If we use the equation (D.27) and write the ξ behind the exponential as $(\mathfrak{M}\bar{\boldsymbol{\xi}})_0 = \int \mathrm{d}\theta e^{\theta(\mathfrak{M}\bar{\xi})_0} = \int \mathrm{d}\theta e^{\theta \mathfrak{M}_{0l} \bar{\xi}_l}$, where θ is a new Grassmann variables. We can write the density matrix as

$$\varrho^\beta(2, \boldsymbol{\xi}, \boldsymbol{\xi'}) = |C^\beta|^2 \beta \int \mathrm{d}\theta e^{\theta(\mathfrak{M}\bar{\xi})_0} e^{\frac{1}{2} R_{ij} \bar{\xi}_i \bar{\xi}_j} e^{-\frac{1}{2} R^*_{ij} \xi'_i \xi'_j}. \tag{D.38}$$

Equivalently, If we introduce new Grassmann variables $\boldsymbol{\eta}^T = \begin{pmatrix} \bar{\boldsymbol{\xi}} & \boldsymbol{\xi} \end{pmatrix}$ then we can write the integral as

$$\varrho^\beta(2, \boldsymbol{\xi}, \boldsymbol{\xi'}) = \int \mathrm{d}\theta \mathcal{F}(\bar{\boldsymbol{\xi}}, \boldsymbol{\xi}', \theta) \int \mathbf{D}\boldsymbol{\eta}\, e^{\frac{1}{2}\boldsymbol{\eta}^T \boldsymbol{\mathcal{A}} \boldsymbol{\eta} + \boldsymbol{\lambda}^T \boldsymbol{\eta}}, \tag{D.39}$$

where we have denoted the terms on the left of second integral by $\mathcal{F}(\bar{\boldsymbol{\xi}}, \boldsymbol{\xi}, \theta)$ and

$$\boldsymbol{\lambda}^T = \begin{pmatrix} -\bar{\boldsymbol{\xi}} \mathbf{R}_{12} - \theta(\mathfrak{M}_{\mathbf{2}})_{0l'} & -\boldsymbol{\xi}' \mathbf{R}^*_{12} \end{pmatrix} \tag{D.40}$$

Taking the integration on $\boldsymbol{\eta}$, we have:

$$\varrho^\beta(2, \boldsymbol{\xi}, \boldsymbol{\xi'}) = \frac{\mathcal{C}^\beta}{\beta^*} e^{\frac{1}{2}\begin{pmatrix} \bar{\xi} & \xi' \end{pmatrix} \mathbf{\Omega} \begin{pmatrix} \bar{\xi} \\ \xi' \end{pmatrix}} \int \mathrm{d}\theta e^{\theta\zeta} \tag{D.41}$$

where $\mathbf{\Omega}$ is the same as (7.72b) and $\mathcal{C}^{\beta}$ is given by (7.72a). Then, we can take the integral over the θ above and write the final result as

$$\varrho^{\beta}(2,\boldsymbol{\xi},\boldsymbol{\xi'}) = \frac{\mathcal{C}^{\beta}}{\beta^{*}}\Big(\boldsymbol{\Upsilon}\boldsymbol{\mathcal{A}}^{-1}\boldsymbol{\mathcal{R}}^{T} + \boldsymbol{\Upsilon'}\Big)\boldsymbol{\eta'}e^{\frac{1}{2}\boldsymbol{\eta'}^{T}\mathbf{\Omega}\boldsymbol{\eta'}} \tag{D.42}$$

where $\boldsymbol{\eta'}^{T} = \begin{pmatrix}\bar{\boldsymbol{\xi}} & \boldsymbol{\xi'}\end{pmatrix}$, and Also we have

$$\boldsymbol{\Upsilon} = \begin{bmatrix}\mathfrak{M}_{\mathbf{2}} & \mathbf{0}\end{bmatrix}_{1\times 2L'} \qquad \boldsymbol{\Upsilon'} = \begin{bmatrix}\mathfrak{M}_{\mathbf{1}} & \mathbf{0}\end{bmatrix}_{1\times 2l} \qquad \boldsymbol{\mathcal{R}} = \begin{bmatrix}\mathbf{R}_{12} & 0\\ 0 & \mathbf{R}^{*}_{12}\end{bmatrix}_{2l\times 2L'} \tag{D.43}$$

For the other cross density (third term in equation (D.28)) we have:

$$\varrho^{\beta}(3,\boldsymbol{\xi},\boldsymbol{\xi'}) = \frac{\mathcal{C}^{\beta}}{\beta}\Big(-\boldsymbol{\Upsilon}\boldsymbol{\mathcal{A}}^{-1}\boldsymbol{\mathcal{R}}^{T} + \boldsymbol{\Upsilon'}\Big)\boldsymbol{\eta'}e^{\frac{1}{2}\boldsymbol{\eta'}^{T}\mathbf{\Omega}^{\beta}\boldsymbol{\eta'}} \tag{D.44}$$

which

$$\boldsymbol{\Upsilon} = \begin{bmatrix}\mathbf{0} & \mathfrak{M}_{\mathbf{2}}{}^{*}\end{bmatrix}_{1\times 2L'} \qquad \boldsymbol{\Upsilon'} = \begin{bmatrix}\mathbf{0} & \mathfrak{M}_{\mathbf{1}}{}^{*}\end{bmatrix} \qquad \boldsymbol{\mathcal{R}} = \begin{bmatrix}\mathbf{R}_{12} & 0\\ 0 & \mathbf{R}^{*}_{12}\end{bmatrix}_{2l\times 2L'} \tag{D.45}$$

Putting equations (D.29), (D.35), (D.42) and (D.44) together and moving and reordering some parts we can write the RDM for the state $|\beta\rangle$ as

$$\rho^{\beta}_{\mathbf{1}}(\boldsymbol{\xi},\boldsymbol{\xi'}) = \mathcal{C}_{\beta}\Big[\frac{1}{|\beta|^{2}} + \mathrm{Pf}[\mathbf{\Omega_2}]e^{\frac{1}{2}\begin{pmatrix}\bar{\xi} & \xi'\end{pmatrix}\mathcal{J}\boldsymbol{\omega}^{-1}\mathcal{J}^{T}\begin{pmatrix}\bar{\xi}\\ \xi'\end{pmatrix} + \boldsymbol{\mathcal{K}}^{\beta}\begin{pmatrix}\bar{\xi}\\ \xi'\end{pmatrix}}\Big]e^{\frac{1}{2}(\mathbf{\Omega}_{11})_{ij}\bar{\xi}_i\bar{\xi}_j}e^{\mathcal{Y}_{ij}\bar{\xi}_i\xi'_j}e^{\frac{1}{2}(\mathbf{\Omega}_{22})_{ij}\xi'_i\xi'_j}, \tag{D.46}$$

where $2\boldsymbol{\mathcal{Y}} = \mathbf{\Omega}_{12} - \mathbf{\Omega}_{21}{}^{T}$ and

$$\boldsymbol{\mathcal{K}}^{\beta} = \begin{pmatrix}\frac{1}{\beta^{*}}\mathfrak{M}_{\mathbf{1}} & \frac{1}{\beta}\mathfrak{M}_{\mathbf{1}}{}^{*}\end{pmatrix} + \begin{pmatrix}\frac{1}{\beta^{*}}\mathfrak{M}_{\mathbf{2}} & -\frac{1}{\beta}\mathfrak{M}_{\mathbf{2}}{}^{*}\end{pmatrix}\boldsymbol{\mathcal{A}}^{-1}\begin{pmatrix}\mathbf{R}_{12}{}^{T} & 0\\ 0 & \mathbf{R}_{12}{}^{\dagger}\end{pmatrix} \tag{D.47}$$

To write the RDM in operator format, we have to reorder it. Then, the final result is

$$\begin{aligned}\rho^{\beta}_{\mathbf{1}}(c,c^{\dagger}) = \mathcal{C}_{\beta}e^{\frac{1}{2}(\mathbf{\Omega}_{11})_{ij}c^{\dagger}_i c^{\dagger}_j}\Big[&\frac{1}{|\beta|^{2}}e^{(\ln\frac{\mathbf{\Omega}_{12}-\mathbf{\Omega}_{21}{}^{T}}{2})_{ij}c^{\dagger}_i c_j} + (\boldsymbol{\mathcal{K}}^{\beta}_{1})_k c^{\dagger}_k e^{(\ln\frac{\mathbf{\Omega}_{12}-\mathbf{\Omega}_{21}{}^{T}}{2})_{ij}c^{\dagger}_i c_j}\\ &+ e^{(\ln\frac{\mathbf{\Omega}_{12}-\mathbf{\Omega}_{21}{}^{T}}{2})_{ij}c^{\dagger}_i c_j}(\boldsymbol{\mathcal{K}}^{\beta}_{2})_l c_l\Big]e^{\frac{1}{2}(\mathbf{\Omega}_{22})_{ij}c_i c_j}\\ &+ \mathcal{C}^{\beta}\mathrm{Pf}[\mathbf{\Omega_2}]e^{\frac{1}{2}(\mathbf{\Omega}'_{11})_{ij}c^{\dagger}_i c^{\dagger}_j}e^{(\ln\frac{\mathbf{\Omega}'_{12}-\mathbf{\Omega}'_{21}{}^{T}}{2})_{ij}c^{\dagger}_i c_j}e^{\frac{1}{2}(\mathbf{\Omega}'_{22})_{ij}c_i c_j}.\end{aligned} \tag{D.48}$$

The $\boldsymbol{\mathcal{K}}_1^\beta$ stands for the first block part of vector $\boldsymbol{\mathcal{K}}^\beta$ (and the same argument for $\boldsymbol{\mathcal{K}}_2^\beta$). To find a shorter notation for the $\rho_{\mathbf{1}}^\beta(c,c^\dagger)$ we use the relation [157]

$$e^{\frac{1}{2}\begin{pmatrix}\mathbf{c}^\dagger & \mathbf{c}\end{pmatrix}\boldsymbol{\mathcal{M}_1}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^\dagger\end{pmatrix}} e^{\frac{1}{2}\begin{pmatrix}\mathbf{c}^\dagger & \mathbf{c}\end{pmatrix}\boldsymbol{\mathcal{M}_2}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^\dagger\end{pmatrix}} e^{\frac{1}{2}\begin{pmatrix}\mathbf{c}^\dagger & \mathbf{c}\end{pmatrix}\boldsymbol{\mathcal{M}_3}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^\dagger\end{pmatrix}} = e^{\frac{1}{2}\begin{pmatrix}\mathbf{c}^\dagger & \mathbf{c}\end{pmatrix}\boldsymbol{\mathcal{M}}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^\dagger\end{pmatrix}} \tag{D.49}$$

where $e^{\boldsymbol{\mathcal{M}}} = e^{\boldsymbol{\mathcal{M}_1}}\, e^{\boldsymbol{\mathcal{M}_2}}\, e^{\boldsymbol{\mathcal{M}_3}}$. Therefore, we can write (D.48) as

$$\begin{aligned}\rho_{\mathbf{1}}^\beta(c,c^\dagger) = \mathcal{C}_\beta \Bigg[\frac{1}{|\beta|^2} e^{\frac{1}{2}\begin{pmatrix}\mathbf{c}^\dagger & \mathbf{c}\end{pmatrix}\boldsymbol{\mathcal{M}}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^\dagger\end{pmatrix}} e^{\frac{1}{2}\operatorname{tr}\ln \boldsymbol{\mathcal{Y}}} + \operatorname{Pf}[\boldsymbol{\Omega_2}] e^{\frac{1}{2}\begin{pmatrix}\mathbf{c}^\dagger & \mathbf{c}\end{pmatrix}\boldsymbol{\mathcal{M}'}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^\dagger\end{pmatrix}} e^{\frac{1}{2}\operatorname{tr}\ln(\boldsymbol{\mathcal{Y}}+\boldsymbol{\mathcal{Y}})} \\ + (\boldsymbol{\mathcal{K}}_1^\beta)_k c_k^\dagger e^{\frac{1}{2}\begin{pmatrix}\mathbf{c}^\dagger & \mathbf{c}\end{pmatrix}\boldsymbol{\mathcal{M}}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^\dagger\end{pmatrix}} e^{\frac{1}{2}\operatorname{tr}\ln \boldsymbol{\mathcal{Y}}} + e^{\frac{1}{2}\begin{pmatrix}\mathbf{c}^\dagger & \mathbf{c}\end{pmatrix}\boldsymbol{\mathcal{M}}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^\dagger\end{pmatrix}} e^{\frac{1}{2}\operatorname{tr}\ln \boldsymbol{\mathcal{Y}}} (\boldsymbol{\mathcal{K}}_2^\beta)_l c_l \Bigg].\end{aligned} \tag{D.50}$$

To move the exponentials to one side (left or right) of the (D.50), we use the relation (7.76). Therefore, we can write the (D.50) as

$$\begin{aligned}\rho_{\mathbf{1}}^\beta(c,c^\dagger) = \mathcal{C}_\beta\, e^{\frac{1}{2}\begin{pmatrix}\mathbf{c}^\dagger & \mathbf{c}\end{pmatrix}\boldsymbol{\mathcal{M}}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^\dagger\end{pmatrix}} e^{\frac{1}{2}\operatorname{tr}\ln(\frac{1}{2}\boldsymbol{\Omega}_{12}-\frac{1}{2}\boldsymbol{\Omega}_{21}^T)} \Bigg[\frac{1}{|\beta|^2} + \begin{pmatrix}\boldsymbol{\mathcal{L}}_1^\beta & \boldsymbol{\mathcal{L}}_2^\beta\end{pmatrix}\begin{pmatrix}\mathbf{c}^\dagger\\ \mathbf{c}\end{pmatrix}\Bigg] \\ + \mathcal{C}_\beta \operatorname{Pf}[\boldsymbol{\Omega_2}] e^{\frac{1}{2}\begin{pmatrix}\mathbf{c}^\dagger & \mathbf{c}\end{pmatrix}\boldsymbol{\mathcal{M}'}\begin{pmatrix}\mathbf{c}\\ \mathbf{c}^\dagger\end{pmatrix}} e^{\frac{1}{2}\operatorname{tr}\ln(\frac{1}{2}\boldsymbol{\Omega}'_{12}-\frac{1}{2}{\boldsymbol{\Omega}'_{21}}^T)}\end{aligned} \tag{D.51}$$

where we have:

$$\boldsymbol{\mathcal{M}} = \ln\begin{pmatrix} \frac{1}{2}\boldsymbol{\Omega}_{12} - \frac{1}{2}{\boldsymbol{\Omega}_{21}}^T + 2\boldsymbol{\Omega}_{11}(\boldsymbol{\Omega}_{12}^T - \boldsymbol{\Omega}_{21})^{-1}\boldsymbol{\Omega}_{22} & 2\boldsymbol{\Omega}_{11}(\boldsymbol{\Omega}_{12}^T - \boldsymbol{\Omega}_{21})^{-1} \\ 2(\boldsymbol{\Omega}_{12}^T - \boldsymbol{\Omega}_{21})^{-1}\boldsymbol{\Omega}_{22} & 2(\boldsymbol{\Omega}_{12}^T - \boldsymbol{\Omega}_{21})^{-1} \end{pmatrix}, \tag{D.52a}$$

$$\boldsymbol{\mathcal{M}}' = \ln\begin{pmatrix} \frac{1}{2}\boldsymbol{\Omega}'_{12} - \frac{1}{2}{\boldsymbol{\Omega}'_{21}}^T + 2\boldsymbol{\Omega}'_{11}({\boldsymbol{\Omega}'_{12}}^T - {\boldsymbol{\Omega}_{21}}')^{-1}\boldsymbol{\Omega}'_{22} & 2\boldsymbol{\Omega}'_{11}({\boldsymbol{\Omega}'_{12}}^T - \boldsymbol{\Omega}'_{21})^{-1} \\ 2({\boldsymbol{\Omega}'_{12}}^T - \boldsymbol{\Omega}'_{21})^{-1}\boldsymbol{\Omega}'_{22} & 2({\boldsymbol{\Omega}'_{12}}^T - \boldsymbol{\Omega}'_{21})^{-1} \end{pmatrix} \tag{D.52b}$$

$$\boldsymbol{\Omega} = \begin{pmatrix} \mathbf{R}_{11} & 0 \\ 0 & -\mathbf{R}_{11}{}^{*} \end{pmatrix} + \begin{pmatrix} \mathbf{R}_{12} & 0 \\ 0 & \mathbf{R}_{12}{}^{*} \end{pmatrix} \boldsymbol{\mathcal{A}}^{-1} \begin{pmatrix} \mathbf{R}_{12}{}^{T} & 0 \\ 0 & \mathbf{R}_{12}{}^{\dagger} \end{pmatrix}; \qquad \boldsymbol{\mathcal{A}} = \begin{pmatrix} \mathbf{R}_{22} & -\mathbf{I} \\ \mathbf{I} & -\mathbf{R}_{22}^{*} \end{pmatrix} \tag{D.52c}$$

$$\boldsymbol{\Omega}' = \boldsymbol{\Omega} + \boldsymbol{\mathcal{J}}\boldsymbol{\omega}^{-1}\boldsymbol{\mathcal{J}}^{T}, \qquad \boldsymbol{\omega} = \begin{pmatrix} \mathfrak{M}_{\mathbf{2}}^{*}(\boldsymbol{\mathcal{A}}^{-1})_{22}\mathfrak{M}_{2}^{\dagger} & -\mathfrak{M}_{\mathbf{2}}^{*}(\boldsymbol{\mathcal{A}}^{-1})_{21}\mathfrak{M}_{2}^{T} \\ -\mathfrak{M}_{2}(\boldsymbol{\mathcal{A}}^{-1})_{12}\mathfrak{M}_{2}^{\dagger} & \mathfrak{M}_{\mathbf{2}}^{*}(\boldsymbol{\mathcal{A}}^{-1})_{11}\mathfrak{M}_{2}^{T} \end{pmatrix} \tag{D.52d}$$

$$\boldsymbol{\mathcal{J}} = \begin{pmatrix} -\mathbf{R}_{12} & \mathbf{0} \\ \mathbf{0} & -\mathbf{R}_{12}{}^{*} \end{pmatrix} \boldsymbol{\mathcal{A}}^{-1} \begin{pmatrix} \mathbf{0} & \mathfrak{M}_{\mathbf{2}}^{*} \\ -\mathfrak{M}_{2} & \mathbf{0} \end{pmatrix} - \begin{pmatrix} \mathbf{0} & \mathfrak{M}_{\mathbf{1}}^{*} \\ \mathfrak{M}_{1} & \mathbf{0} \end{pmatrix}, \tag{D.52e}$$

$$\boldsymbol{\mathcal{K}}^{\beta} = \begin{pmatrix} \frac{1}{\beta^{*}}\mathfrak{M}_{\mathbf{1}} & \frac{1}{\beta}\mathfrak{M}_{\mathbf{1}}{}^{*} \end{pmatrix} + \begin{pmatrix} \frac{1}{\beta^{*}}\mathfrak{M}_{\mathbf{2}} & -\frac{1}{\beta}\mathfrak{M}_{\mathbf{2}}{}^{*} \end{pmatrix} \boldsymbol{\mathcal{A}}^{-1} \begin{pmatrix} \mathbf{R}_{12}{}^{T} & 0 \\ 0 & \mathbf{R}_{12}{}^{\dagger} \end{pmatrix} \tag{D.52f}$$

$$\boldsymbol{\mathcal{L}}_{1}^{\beta} = 2\boldsymbol{\mathcal{K}}_{1}^{\beta}(\boldsymbol{\Omega}_{12}^{T} - \boldsymbol{\Omega}_{21})^{-1}, \qquad \boldsymbol{\mathcal{L}}_{2}^{\beta} = 2\boldsymbol{\mathcal{K}}_{1}^{\beta}(\boldsymbol{\Omega}_{12}^{T} - \boldsymbol{\Omega}_{21})^{-1}\boldsymbol{\Omega}_{22} + \boldsymbol{\mathcal{K}}_{2}^{\beta}. \tag{D.52g}$$

$\boldsymbol{\mathcal{K}}_{1}^{\beta}$ stands for the first block part of vector $\boldsymbol{\mathcal{K}}^{\beta}$. Since, we can think of $\boldsymbol{\mathcal{K}}^{\beta}$ as a vector made from two block vectors (and the same argument for $\boldsymbol{\mathcal{K}}_{2}^{\beta}$).

Entanglement calculations of general β parity broken state

To calculate the $n = 2$ Rényi EE, we start by:

$$\mathrm{tr}(\rho_{A}^{\beta\,2}) = \mathrm{tr}(\rho_{A}^{\beta}\mathbf{I}\rho_{A}^{\beta}). \tag{D.53}$$

We can use the Identity resolution and tracing formula of Grassmann variables to write:

$$\mathbf{I} = \int \prod_{l} \mathrm{d}\bar{\xi}_{l}\mathrm{d}\xi_{l} e^{-\bar{\boldsymbol{\xi}}.\boldsymbol{\xi}} \left|\boldsymbol{\xi}\right\rangle\left\langle\boldsymbol{\xi}\right|, \tag{D.54a}$$

$$\mathrm{tr}\mathcal{O} = \int \prod_{i} \mathrm{d}\bar{\xi}_{i}\mathrm{d}\xi_{i} e^{-\bar{\boldsymbol{\xi}}.\boldsymbol{\xi}} \left\langle -\boldsymbol{\xi}\right| \mathcal{O} \left|\boldsymbol{\xi}\right\rangle. \tag{D.54b}$$

Therefore, it is possible to calculate the trace of ρ^2 in terms of Berezin integrals of Grassmann variables:

$$\mathrm{tr}(\rho_{A}^{\beta\,2}) = \int \prod_{i} \mathrm{d}\bar{\xi}_{i}\mathrm{d}\xi_{i} \prod_{l} \mathrm{d}\bar{\eta}_{l}\mathrm{d}\eta_{l} e^{-\bar{\boldsymbol{\xi}}.\boldsymbol{\xi}} e^{-\bar{\boldsymbol{\eta}}.\boldsymbol{\eta}} \left\langle -\boldsymbol{\xi}\right| \rho_{A}^{\beta} \left|\boldsymbol{\eta}\right\rangle\left\langle\boldsymbol{\eta}\right| \rho_{A}^{\beta} \left|\boldsymbol{\xi}\right\rangle. \tag{D.55}$$

We can use the result of (7.71) to write the integrand in the expression above as:

$$\begin{aligned}\mathrm{tr}(\rho_A^{\beta\,2}) =&\mathcal{C}^{\beta^2}\int\prod_i \mathrm{d}\bar{\xi}_i\mathrm{d}\xi_i\prod_l \mathrm{d}\bar{\eta}_l\mathrm{d}\eta_l e^{-\bar{\boldsymbol{\xi}}.\boldsymbol{\xi}}e^{-\bar{\boldsymbol{\eta}}.\boldsymbol{\eta}}[(\frac{1}{\beta}-\boldsymbol{\mathcal{L}}_1.\bar{\boldsymbol{\xi}}+\boldsymbol{\mathcal{L}}_2.\boldsymbol{\eta})(\frac{1}{\beta^*}-\boldsymbol{\mathcal{L}}_3.\bar{\boldsymbol{\xi}}+\boldsymbol{\mathcal{L}}_4.\boldsymbol{\eta})-\mathrm{Pf}[\boldsymbol{\mathcal{W}}]]\\ &e^{\frac{1}{2}\begin{pmatrix}\bar{\xi} & \eta\end{pmatrix}\boldsymbol{\Omega}'\begin{pmatrix}\bar{\xi}\\ \eta\end{pmatrix}}[(\frac{1}{\beta}+\boldsymbol{\mathcal{L}}_1.\bar{\boldsymbol{\eta}}+\boldsymbol{\mathcal{L}}_2.\boldsymbol{\xi})(\frac{1}{\beta^*}+\boldsymbol{\mathcal{L}}_3.\bar{\boldsymbol{\eta}}+\boldsymbol{\mathcal{L}}_4.\boldsymbol{\xi})-\mathrm{Pf}[\boldsymbol{\mathcal{W}}]]e^{\frac{1}{2}\begin{pmatrix}\bar{\eta} & \xi\end{pmatrix}\boldsymbol{\Omega}\begin{pmatrix}\bar{\eta}\\ \xi\end{pmatrix}},\end{aligned} \tag{D.56}$$

By defining a new Grassmann variable such as:

$$\boldsymbol{\theta}=\begin{pmatrix}\bar{\boldsymbol{\xi}}\\ \bar{\boldsymbol{\eta}}\\ \boldsymbol{\eta}\\ \boldsymbol{\xi}\end{pmatrix}, \tag{D.57}$$

the integral (D.55) can be written in a simpler form as:

$$\mathrm{tr}(\rho_A^{\beta\,2})=\mathcal{C}^{\beta^2}\int\mathbf{D}\boldsymbol{\theta}\mathrm{f}(\boldsymbol{\theta})e^{\frac{1}{2}\boldsymbol{\theta}^T.\boldsymbol{\mathcal{B}}.\boldsymbol{\theta}}, \tag{D.58}$$

where in the above $\mathbf{D}\boldsymbol{\theta}=\prod_i \mathrm{d}\bar{\theta}_i\mathrm{d}\theta_i$, and also

$$\mathrm{f}(\boldsymbol{\theta})=\Big[(\frac{1}{\beta}+\mathbb{C}.\boldsymbol{\theta}|_1)(\frac{1}{\beta^*}+\mathbb{C}.\boldsymbol{\theta}|_2)+\mathrm{Pf}[\boldsymbol{\mathcal{W}}]\Big]\Big[(\frac{1}{\beta}+\mathbb{C}.\boldsymbol{\theta}|_3)(\frac{1}{\beta^*}+\mathbb{C}.\boldsymbol{\theta}|_4)+\mathrm{Pf}[\boldsymbol{\mathcal{W}}]\Big].$$

The new $\boldsymbol{\mathcal{B}}$ and $\mathbb{C}$ matrices are defined below

$$\boldsymbol{\mathcal{B}}=\begin{pmatrix}\boldsymbol{\Omega}_{11} & \mathbf{0} & -\boldsymbol{\Omega}_{12} & \mathbf{I}\\ \mathbf{0} & \boldsymbol{\Omega}_{11} & \mathbf{I} & \boldsymbol{\Omega}_{12}\\ -\boldsymbol{\Omega}_{21} & -\mathbf{I} & \boldsymbol{\Omega}_{22} & \mathbf{0}\\ -\mathbf{I} & \boldsymbol{\Omega}_{21} & \mathbf{0} & \boldsymbol{\Omega}_{21}\end{pmatrix},\qquad \mathbb{C}=\begin{pmatrix}-\boldsymbol{\mathcal{L}}_1 & \mathbf{0} & \boldsymbol{\mathcal{L}}_2 & \mathbf{0}\\ -\boldsymbol{\mathcal{L}}_3 & \mathbf{0} & \boldsymbol{\mathcal{L}}_4 & \mathbf{0}\\ \mathbf{0} & \boldsymbol{\mathcal{L}}_1 & \mathbf{0} & \boldsymbol{\mathcal{L}}_2\\ \mathbf{0} & \boldsymbol{\mathcal{L}}_3 & \mathbf{0} & \boldsymbol{\mathcal{L}}_4\end{pmatrix}. \tag{D.59}$$

The rest of matrices are given by (7.72). Before proceeding to solve the integral above, we have to clarify couple of points here. First, the notation $\mathbb{C}.\boldsymbol{\theta}|_r$ stand for the r^{th} row of the matrix product $\mathbb{C}.\boldsymbol{\theta}$. Second, the $\mathrm{f}(\boldsymbol{\theta})$ produce terms with product of odd number of Grassmann variables such as $\mathbb{C}.\boldsymbol{\theta}|_r$ or $\mathbb{C}.\boldsymbol{\theta}|_{r_3}\mathbb{C}.\boldsymbol{\theta}|_{r_2}\mathbb{C}.\boldsymbol{\theta}|_{r_1}$, the integration on these terms will be zero automatically. Therefore, The above integral is straightforward to solve, and the final result of tracing is given by (7.102).

In some cases $\boldsymbol{\mathcal{B}}$ does not have an inverse for odd n. However, it is still possible to take the Grassmann integrations.

Exact diagonalization of $\mathbf{A} = \mathbf{B} = 0$

In the case where $\mathbf{A}$ and $\mathbf{B}$ are zero then the Hamiltonian (7.5) becomes

$$H = \sum_{j=1}^{L} \Big[\alpha_j^0(c_0 c_j - c_0^\dagger c_j) + \alpha_j^{L+1}(c_j c_{L+1}^\dagger + c_j c_{L+1}) + \alpha_j^{0*}(c_j^\dagger c_0^\dagger - c_j^\dagger c_0) + \alpha_j^{L+1*}(c_{L+1} c_j^\dagger + c_{L+1}^\dagger c_j^\dagger)\Big]. \tag{D.60}$$

This model can be related to a linear fermionic model such as the model discussed in [152]

$$H = \sum_{j=1}^{L} \alpha_j c_j + \alpha_j^* c_j^\dagger. \tag{D.61}$$

In fact, with a specific projection, one can find the eigenstates of (D.61) in the Hilbert space of (D.60). We can write the new form of the $\mathbf{M}$ matrix (7.9)

$$
\mathbf{M} = \left(\begin{array}{ccccccc|ccccccc}
0 & -\alpha_1^0 & -\alpha_2^0 & \cdots & -\alpha_{L-1}^0 & -\alpha_L^0 & 0 & 0 & -\alpha_1^{0*} & -\alpha_2^{0*} & \cdots & -\alpha_{L-1}^{0\ *} & -\alpha_L^{0*} & 0 \\
-\alpha_1^{0*} & 0 & 0 & \cdots & 0 & 0 & -\alpha_1^{L+1*} & \alpha_1^{0*} & 0 & 0 & \cdots & 0 & 0 & -\alpha_1^{L+1*} \\
-\alpha_2^{0*} & 0 & 0 & & & 0 & -\alpha_2^{L+1*} & \alpha_2^{0*} & 0 & & & & 0 & -\alpha_2^{L+1*} \\
\vdots & \vdots & & & & & \vdots & \vdots & \vdots & & & & \cdots & \vdots \\
-\alpha_{L-1}^{0\ *} & 0 & & & & 0 & -\alpha_{L-1}^{L+1*} & \alpha_{L-1}^{0\ *} & 0 & & & & 0 & -\alpha_{L-1}^{L+1*} \\
-\alpha_L^{0*} & 0 & 0 & \cdots & 0 & 0 & -\alpha_L^{L+1*} & \alpha_L^{0*} & 0 & 0 & \cdots & 0 & 0 & -\alpha_L^{L+1*} \\
\hline
0 & -\alpha_1^{L+1} & -\alpha_2^{L+1} & \cdots & -\alpha_{L-1}^{L+1} & -\alpha_L^{L+1} & 0 & 0 & \alpha_1^{L+1*} & \alpha_2^{L+1*} & \cdots & \alpha_{L-1}^{L+1*} & \alpha_L^{L+1*} & 0 \\
0 & \alpha_1^0 & \alpha_2^0 & \cdots & \alpha_{L-1}^0 & \alpha_L^0 & 0 & 0 & \alpha_1^{0*} & \alpha_2^{0*} & \cdots & \alpha_{L-1}^{0\ *} & \alpha_L^{0*} & 0 \\
-\alpha_1^0 & 0 & 0 & \cdots & 0 & 0 & \alpha_1^{L+1} & \alpha_1^0 & 0 & 0 & \cdots & 0 & 0 & \alpha_1^{L+1} \\
-\alpha_2^0 & 0 & 0 & & & 0 & \alpha_2^{L+1} & \alpha_2^0 & 0 & & & & 0 & \alpha_2^{L+1} \\
\vdots & \vdots & & & & & \vdots & \vdots & \vdots & & & & \cdots & \vdots \\
-\alpha_{L-1}^0 & 0 & & & & 0 & \alpha_{L-1}^{L+1} & \alpha_{L-1}^0 & 0 & & & & 0 & \alpha_{L-1}^{L+1} \\
-\alpha_L^0 & 0 & 0 & \cdots & 0 & 0 & \alpha_L^{L+1} & \alpha_L^0 & 0 & 0 & \cdots & 0 & 0 & \alpha_L^{L+1} \\
0 & -\alpha_1^{L+1} & -\alpha_2^{L+1} & \cdots & -\alpha_{L-1}^{L+1} & -\alpha_L^{L+1} & 0 & 0 & \alpha_1^{L+1*} & \alpha_2^{L+1*} & \cdots & \alpha_{L-1}^{L+1*} & \alpha_L^{L+1*} & 0
\end{array}\right)
\tag{D.62}
$$

.

It can be shown that $\mathbf{\Lambda}$ has only two nonzero diagonal elements, λ_1 and λ_2 and the rest of eigenvalues are zero. For nonzero eigenvalues, we have

$$\lambda_1, \lambda_2 = \sqrt{2}\sqrt{\sum_{j=1}^{L}(|\alpha_j^0|^2 + |\alpha_j^{L+1}|^2) \pm \sqrt{\left|\sum_{j=1}^{L}(\alpha_j^0 + \alpha_j^{L+1})(\alpha_j^{0*} - \alpha_j^{L+1*})\right|^2}}. \tag{D.63}$$

Then, $\mathbf{M}$ would have only four nonzero eigenvalues and the rest are zero independent of size. The next step is to find the eigenvectors to construct the $\mathbf{U}$ matrix. In (7.12), we have already introduced two eigenvectors of zero mode. Using the orthogonality condition, and the condition that if $|u\rangle$ is an eigenvector with eigenvalue λ then $\mathbf{J}|u\rangle$ is also an eigenvector with eigenvalue $-\lambda$, therefore, we can find and present only half of the eigenvectors. For simplicity, we assume $\alpha_j^0 = \alpha_j^{L+1} = \alpha_j$, then eigenvectros of positive modes. we have:

$$\left|u_1^+\right\rangle = \begin{pmatrix} u \\ \\ v \end{pmatrix}; \qquad \begin{aligned} &u_{L+1} = u_0 = -v_0 = v_{L+1} = 1 \\ &u_i = -\frac{2\alpha_i^*}{\sqrt{\sum_{j=1}^{L}|\alpha_j|^2}} \\ &\text{else} = 0 \end{aligned} \tag{D.64}$$

$$\left|u_2^+\right\rangle = \begin{pmatrix} u \\ \\ v \end{pmatrix}; \qquad \begin{aligned} &u_{L+1} = -u_0 = v_0 = v_{L+1} = \frac{\alpha_L}{|\alpha_L|} \\ &v_i = \frac{2\alpha_i}{\sqrt{\sum_{j=1}^{L}|\alpha_j|^2}}\frac{\alpha_L}{|\alpha_L|} \\ &\text{else} = 0 \end{aligned} \tag{D.65}$$

For eigenvectros of zero modes, we have:

$$\left|u_1^0\right\rangle = \begin{pmatrix} u \\ \\ v \end{pmatrix}; \qquad \begin{aligned} &u_{L+1} = u_0 = v_0 = -v_{L+1} = 1 \\ &\text{else} = 0 \end{aligned} \tag{D.66}$$

$$\left|u_k^0\right\rangle = \begin{pmatrix} u \\ \\ v \end{pmatrix}; \qquad \begin{aligned} &u_i = -\frac{\alpha_k\alpha_i^*}{\sum_{j=1}^{k-1}|\alpha_j|^2}; \quad i < k \neq 0 \\ &u_k = 1 \\ &\text{else} = 0, \end{aligned} \tag{D.67}$$

where $k = 2, 3, \cdots, L$. With this expressions for eigenvectors, we can construct the unitary matrices $\mathbf{U}$. Having the exact $\mathbf{U}$, we can calculate correlation matrices (see section 7.3). putting these eigenvectors together, one can construct the $\mathbf{U}$.

Having the $\mathbf{U}$ matrix, we can directly calculate the δ_+ introduced in (7.35). The calculation of δ_+ shows that

$$\delta_+ = \begin{cases} +1 & \text{if } L \text{ even} \\ -1 & \text{if } L \text{ odd} \end{cases} \tag{D.68}$$

Vacuum state in configuration basis

Another method to calculate the entanglement of subsystem in a particular state is to use a more direct way. We could use the equation (2.53) to calculate the entanglement. Using the results of subsection 7.2.4 for $\mathbf{A}, \mathbf{B} = 0$ we can find the form of $\mathbf{R}$ matrix as:.

$$\mathbf{R} = \left(\begin{array}{c|c|c} 0 & \frac{\alpha_j}{\sqrt{|\alpha_1|^2+\cdots+|\alpha_L|^2}} & 1 \\ \hline \frac{-\alpha_i}{\sqrt{|\alpha_1|^2+\cdots+|\alpha_L|^2}} & 0 & \frac{\alpha_i}{\sqrt{|\alpha_1|^2+\cdots+|\alpha_L|^2}} \\ \hline -1 & \frac{-\alpha_j}{\sqrt{|\alpha_1|^2+\cdots+|\alpha_L|^2}} & 0 \end{array}\right) \tag{D.69}$$

where,

$$|0\rangle_\eta = \frac{1}{\sqrt{\det[\mathbf{I}+\mathbf{R}^\dagger\mathbf{R}]}} e^{\frac{1}{2}\sum_{i,j} R_{ij} c_i^\dagger c_j^\dagger} |0\rangle_c .$$

Numerical investigations suggest that for even sizes we get exactly the same expression, and for odd sizes we get the minus of the vacuum ($\alpha_i \in \mathbb{R}$).

Correlations

For the special case of $\mathbf{A}, \mathbf{B} = 0$, the correlation matrices look pretty much simple in terms of the parameters α_i's. We are going to demonstrate the matrix form of correlations for general $\alpha_i \in \mathbb{C}$. For start, in the vacuum state, correlations looks like below. (In the following expressions indexes n and m are the number of rows and columns respectively.)

$$\mathbf{C}^0 = \left(\begin{array}{c|c|c} \frac{1}{2} & \frac{\alpha_m}{4\sqrt{\sum_k |\alpha_k|^2}} & -\frac{1}{4} \\ \hline \frac{\alpha_n^*}{4\sqrt{\sum_k |\alpha_k|^2}} & \frac{\alpha_n^*\alpha_m}{2(\sum_k |\alpha_k|^2)} & \frac{\alpha_n^*}{4\sqrt{\sum_k |\alpha_k|^2}} \\ \hline -\frac{1}{4} & \frac{\alpha_m}{4\sqrt{\sum_k |\alpha_k|^2}} & \frac{1}{2} \end{array}\right), \quad \mathbf{F}^0 = \left(\begin{array}{c|c|c} 0 & \frac{\alpha_m^*}{4\sqrt{\sum_k |\alpha_k|^2}} & \frac{1}{4} \\ \hline \frac{-\alpha_n^*}{4\sqrt{\sum_k |\alpha_k|^2}} & 0 & \frac{\alpha_n^*}{4\sqrt{\sum_k |\alpha_k|^2}} \\ \hline -\frac{1}{4} & \frac{-\alpha_m^*}{4\sqrt{\sum_k |\alpha_k|^2}} & 0 \end{array}\right)$$

$$\mathbf{K}^0 = \left(\begin{array}{c|c|c} 1 & 0 & 0 \\ \hline 0 & \delta_{nm} - \frac{m-n}{|m-n|} \frac{i\Im[\alpha_n^*\alpha_m]}{\sum_k |\alpha_k|^2} & \frac{-i\Im[\alpha_n]}{\sqrt{\sum_k |\alpha_k|^2}} \\ \hline 0 & \frac{i\Im[\alpha_m]}{\sqrt{\sum_k |\alpha_k|^2}} & 1 \end{array}\right), \quad \bar{\mathbf{K}}^0 = \left(\begin{array}{c|c|c} 1 & \frac{i\Im[\alpha_m]}{\sqrt{\sum_k |\alpha_k|^2}} & 0 \\ \hline \frac{-i\Im[\alpha_n]}{\sqrt{\sum_k |\alpha_k|^2}} & \delta_{nm} - \frac{m-n}{|m-n|} \frac{i\Im[\alpha_n^*\alpha_m]}{\sum_k |\alpha_k|^2} & 0 \\ \hline 0 & 0 & 1 \end{array}\right)$$

$$\mathbf{G}^0 = \left(\begin{array}{c|c|c} 0 & \frac{\Re[\alpha_m]}{\sqrt{\sum_k |\alpha_k|^2}} & 0 \\ \hline 0 & -\delta_{nm} + \frac{\Re[\alpha_n^* \alpha_m]}{\sum_k |\alpha_k|^2} & \frac{\Re[\alpha_n]}{\sqrt{\sum_k |\alpha_k|^2}} \\ \hline -1 & 0 & 0 \end{array}\right)$$

For the case where the state is ZME state ($|\emptyset\rangle$) then the correlation matrices look like below.

$$\mathbf{C}^{\emptyset} = \left(\begin{array}{c|c|c} \frac{1}{2} & \frac{\alpha_m}{4\sqrt{\sum_k |\alpha_k|^2}} & \frac{1}{4} \\ \hline \frac{\alpha_n^*}{4\sqrt{\sum_k |\alpha_k|^2}} & \frac{\alpha_n^* \alpha_m}{2(\sum_k |\alpha_k|^2)} & \frac{\alpha_n^*}{4\sqrt{\sum_k |\alpha_k|^2}} \\ \hline \frac{1}{4} & \frac{\alpha_m}{4\sqrt{\sum_k |\alpha_k|^2}} & \frac{1}{2} \end{array}\right), \quad \mathbf{F}^{\emptyset} = \left(\begin{array}{c|c|c} 0 & \frac{\alpha_m^*}{4\sqrt{\sum_k |\alpha_k|^2}} & -\frac{1}{4} \\ \hline \frac{-\alpha_n^*}{4\sqrt{\sum_k |\alpha_k|^2}} & 0 & \frac{\alpha_n^*}{4\sqrt{\sum_k |\alpha_k|^2}} \\ \hline \frac{1}{4} & \frac{-\alpha_m^*}{4\sqrt{\sum_k |\alpha_k|^2}} & 0 \end{array}\right)$$

$$\mathbf{G}^{\emptyset} = \left(\begin{array}{c|c|c} 0 & \frac{\Re[\alpha_m]}{\sqrt{\sum_k |\alpha_k|^2}} & 0 \\ \hline 0 & -\delta_{nm} + \frac{\Re[\alpha_n^* \alpha_m]}{\sum_k |\alpha_k|^2} & \frac{\Re[\alpha_n]}{\sqrt{\sum_k |\alpha_k|^2}} \\ \hline 1 & 0 & 0 \end{array}\right), \qquad \mathbf{K}^{\emptyset} = \mathbf{K}^0, \qquad \bar{\mathbf{K}}^{\emptyset} = \bar{\mathbf{K}}^0.$$

Finally, for this case when the state is $|G_{\pm}\rangle$ then the correlations look like below.

$$\mathbf{C}^{\pm} = \left(\begin{array}{c|c|c} \frac{1}{2} & \frac{\alpha_m}{4\sqrt{\sum_k |\alpha_k|^2}} & 0 \\ \hline \frac{\alpha_n^*}{4\sqrt{\sum_k |\alpha_k|^2}} & \frac{\alpha_n^* \alpha_m}{2(\sum_k |\alpha_k|^2)} & \frac{\alpha_n^*}{4\sqrt{\sum_k |\alpha_k|^2}} \\ \hline 0 & \frac{\alpha_m}{4\sqrt{\sum_k |\alpha_k|^2}} & \frac{1}{2} \end{array}\right), \quad \mathbf{F}^{\pm} = \left(\begin{array}{c|c|c} 0 & \frac{\alpha_m^*}{4\sqrt{\sum_k |\alpha_k|^2}} & 0 \\ \hline \frac{-\alpha_n^*}{4\sqrt{\sum_k |\alpha_k|^2}} & 0 & \frac{\alpha_n^*}{4\sqrt{\sum_k |\alpha_k|^2}} \\ \hline 0 & \frac{-\alpha_m^*}{4\sqrt{\sum_k |\alpha_k|^2}} & 0 \end{array}\right),$$

$$\mathbf{G}^{\pm} = \left(\begin{array}{c|c|c} 0 & \frac{\Re[\alpha_m]}{\sqrt{\sum_k |\alpha_k|^2}} & 0 \\ \hline 0 & -\delta_{nm} + \frac{\Re[\alpha_n^* \alpha_m]}{\sum_k |\alpha_k|^2} & \frac{\Re[\alpha_n]}{\sqrt{\sum_k |\alpha_k|^2}} \\ \hline 0 & 0 & 0 \end{array}\right), \qquad \mathbf{K}^{\pm} = \mathbf{K}^0, \qquad \bar{\mathbf{K}}^{\pm} = \bar{\mathbf{K}}^0.$$

M matrix for modified XY chain

In this appendix, the exact forms of the matrices **A** and **B** for modified XY spin chain is demonstrated. For $|\vec{b}_1| = 1$ and $|\vec{b}_L| = 1$, they can be written as:

$$\mathbf{A} = \begin{pmatrix} 0 & -\frac{\sin\theta_1 e^{i\phi_1}}{2} & 0 & ... & & & & \\ -\frac{\sin\theta_1 e^{-i\phi_1}}{2} & -h+\cos\theta_1 & -\frac{J}{2} & 0 & ... & & & \\ 0 & -\frac{J}{2} & -h & -\frac{J}{2} & 0 & ... & & \\ 0 & 0 & -\frac{J}{2} & -h & -\frac{J}{2} & 0 & ... & \\ . & . & . & & & & & \\ . & . & . & & & & & \\ & & & & . & . & -h+\cos\theta_L & -\frac{\sin\theta_L e^{-i\phi_L}}{2} \\ & & & & \cdots & 0 & -\frac{\sin\theta_L e^{i\phi_L}}{2} & 0 \end{pmatrix}, \quad \text{(D.70)}$$

$$\mathbf{B} = \begin{pmatrix} 0 & -\frac{\sin\theta_1 e^{-i\phi_1}}{2} & 0 & \cdots & & & & & \\ \frac{\sin\theta_1 e^{-i\phi_1}}{2} & 0 & -\frac{J\gamma}{2} & 0 & \cdots & & & & \\ 0 & \frac{J\gamma}{2} & 0 & -\frac{\gamma J}{2} & 0 & ... & & & \\ \vdots & 0 & \frac{J\gamma}{2} & 0 & -\frac{\gamma J}{2} & 0 & ... & & \\ & . & . & & & & & & \\ & . & . & & & & & & \\ & . & . & . & . & . & \frac{J\gamma}{2} & 0 & -\frac{\sin\theta_L e^{-i\phi_L}}{2} \\ & . & . & . & . & . & 0 & \frac{\sin\theta_L e^{-i\phi_L}}{2} & 0 \end{pmatrix}. \quad \text{(D.71)}$$

With the help of (7.8) and (7.9), one can construct the actual **M** matrix.