Entanglement Spectra and Boundary Theories for Gaussian Fermionic PEPS

von

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Masterarbeit in Physik

vorgelegt

der Fakultät für Mathematik, Informatik und Naturwissenschaften der RWTH Aachen

im Oktober 2013

angefertigt im

Institut für Quanteninformation

bei

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Ich, Stefan Thomas Haßler, versichere, dass ich die Masterarbeit "Entanglement spectra and boundary theories for Gaussian fermionic PEPS" selbstständig verfasst und keine anderen als die angegebenen Quellen und Hilfsmittel benutzt, sowie Zitate kenntlich gemacht habe.

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Abstract

In this thesis, we will investigate Gaussian fermionic Projected Entangled Pair States (GfPEPS). The GfPEPS formalism is a natural generalization of the PEPS construction for spin systems to fermionic Gaussian states. We will consider fermionic Gaussian states of a 2-dimensional system of fermionic modes on a cylinder. The GfPEPS gives a good approximation to these systems and they can be described very efficiently with their corresponding covariance matrix.

In [1], it was shown for PEPS that there is a mapping between the physical spin system of a reduced state and its auxiliary system at the boundary. We will show that we can also find such a mapping for a reduced GfPEPS. This implies that the entanglement spectrum, associated to the reduced state of a region of the GfPEPS, is directly related to the spectrum of the virtual modes at the boundary of this region.

Therefore, we will investigate the behavior of the auxiliary system in the GfPEPS construction. We are able to show for certain situations that the virtual modes on both edges of the auxiliary system decouple for increasing system lengths and that the coupling decays exponentially with the number of sites in horizontal direction. We will show this behavior for some examples and relate the resulting boundary spectrum to the entanglement spectrum for these examples.

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1. Introduction

Correlated quantum many-body systems are of great interest in condensed matter physics. Such systems show very interesting properties such as superconductivity or topological order. But the accurate description and numerical simulation of strongly correlated quantum many-body systems is a very difficult task in modern condensed matter physics.

The introduction of Matrix Product States (MPS) in recent years gave a good insight in such complex systems. For spin systems in one spatial dimension, MPS are suitable to give good approximations to the ground state of any gapped Hamiltonian [2, 3]. Since the powerful DMRG (Density Matrix Renormalization Group) algorithm can be seen as a variational method in the MPS formalism [2], these states are also very powerful for numerical simulations. A natural generalization to more than one spatial dimensions is done with Projected Entangled Pair States (PEPS) which give good approximations to spin systems with local interactions at finite temperatures [3, 4]. PEPS were introduced to efficiently simulate two-dimensional systems, since the generalization of the DMRG algorithm in more than one dimension shows no good scaling [2]. For example, it was possible to give exact approximations to some topological states in 2D using PEPS constructions [4]. If one wants to describe systems of fermions on a lattice now, one has to pay attention to the anti-commutation relations of the fermionic operators. Therefore, fermionic PEPS (fPEPS) were introduced in [3]. They naturally extend the PEPS construction to fermionic systems and respect these anti-commutation relations.

Another interesting discovery was made in the context of entanglement spectra. If we divide a state into two regions and calculate the reduced density matrix for region 1, then we can assign a Hamiltonian to that reduced state. The spectrum of this Hamiltonian is called the entanglement spectrum and for certain models in two spatial dimensions it shows only a 1-dimensional behavior [1]. This clear mismatch in dimensions seems to reflect the so called area law: Instead of being dependent on all possible states in the volume of that region, the entanglement spectrum only depends on the states at the boundary of the region. For PEPS, it was possible to give a very intuitive interpretation to this behavior: the entanglement spectrum of a reduced PEPS is directly connected to the spectrum of the virtual particles at the boundary between the two regions [1].

In this thesis, we will investigate Gaussian fermionic Projected Entangled Pair States (GfPEPS) which are used to describe a fermionic Gaussian state of fermionic modes on a two-dimensional lattice. In chapter 2, we will give an overview on fermionic Gaussian states and their properties. We will present the important connection between the covariance matrix and the Hamiltonian

of such states. Then, we want to consider a fermionic Gaussian state of fermionic modes on a cylinder and describe it by a GfPEPS. After a brief overview on the PEPS construction of a system of spins on a square lattice, we will naturally extend this construction to the GfPEPS case. In chapter 3, we will investigate the entanglement spectrum for GfPEPS. We will show that the entanglement spectrum for a reduced GfPEPS of a region 1 is directly connected to the virtual particles at the boundary of that region, similar to [1]. Chapter 4 will focus on the auxiliary system of a GfPEPS. We will show for certain systems that the virtual particles on the left and right boundary decouple for increasing horizontal length. For some special cases, we will prove that this coupling decays exponentially with the number of sites in horizontal direction. We will give expressions for the diagonal entries of the covariance matrix which describes the auxiliary state in the limit of large auxiliary systems. Finally, in chapter 5, we will present three numerical examples for GfPEPS and discuss the properties of their auxiliary system.

2. Fermionic Systems

In this chapter we want to describe the construction of Gaussian fermionic Projected Entangled Pair States (GfPEPS). To this end, we first explain how to describe fermionic systems. We introduce fermionic Gaussian states and various ways to describe them and how to do calculations with them. After a brief overview on Projected Entangled Pair States (PEPS) for spins on a lattice, we want to focus on GfPEPS on a cylinder.

Let us consider a system of *n* fermions with creation and annihilation operators a_j^{\dagger} and a_j (j = 1...n), respectively, which satisfy the fermionic anti-commutation relations $\{a_j, a_k\} = \{a_j^{\dagger}, a_k^{\dagger}\} = 0$ and $\{a_j, a_k^{\dagger}\} = \delta_{jk}$. A state of *n* fermions can be described in the Fock basis [5, 6]

$$|N_1, \dots, N_n\rangle = \left(a_1^{\dagger}\right)^{N_1} \dots \left(a_n^{\dagger}\right)^{N_n} |0\rangle, \qquad (2.1)$$

where $N_j \in \{0, 1\}$ is the occupation number of the j – th fermionic mode and $|0\rangle$ is the fermionic vacuum which satisfies $a_j |0\rangle = 0$.

For the description of fermionic Gaussian states it is convenient to introduce 2n so called Majorana operators

$$c_{2j-1} = a_j^{\dagger} + a_j \text{ and } c_{2j} = -i \left(a_j^{\dagger} - a_j \right)$$
 (2.2)

which form a Clifford algebra $\{c_k, c_l\} = 2\delta_{kl}\mathbb{1}$, wherein $k, l \in \{1, \ldots, 2n\}$. We will call the c_{2j-1} odd and the c_{2j} even Majorana operators.

2.1. Fermionic Gaussian States

2.1.1. Definition of Fermionic Gaussian States

Now we want to define fermionic Gaussian states. Let us start with the density matrix of a system of n fermions in the canonical ensemble [7, p. 118], which is given by

$$\boldsymbol{\rho} = \frac{1}{\mathrm{Tr}\left(\mathrm{e}^{-\beta \mathcal{H}}\right)} \,\mathrm{e}^{-\beta \mathcal{H}} \tag{2.3}$$

where β is the inverse temperature and **H** is the Hamiltonian of the system.

We want to consider systems that are described by a Hamiltonian that only contains quadratic

terms of Majorana operators [5, 6], i.e.

$$\beta \mathcal{H} = \frac{\mathrm{i}}{4} \boldsymbol{c}^T \boldsymbol{H} \boldsymbol{c} = \frac{\mathrm{i}}{4} \sum_{a,b=1}^{2n} H_{ab} c_a c_b$$

 \boldsymbol{H} is a real, antisymmetric $2n \times 2n$ matrix, due to the Clifford Algebra of the Majorana operators and $\boldsymbol{c} = (c_1, c_2, \dots, c_{2n})^T$ is a vector of Majorana operators. We enclosed the prefactor β in the definition of the matrix \boldsymbol{H} . Systems with such Hamiltonians can be calculated exactly in the fermionic Gaussian state formalism. The density matrix in eq. (2.3) for such a Hamiltonian has the general form

$$\boldsymbol{\rho} = \frac{1}{Z} e^{-\frac{i}{4}\boldsymbol{c}^T \boldsymbol{H} \boldsymbol{c}}$$
(2.4)

with a normalization constant Z.

A system with a density matrix satisfying eq. (2.4) is called a fermionic Gaussian state. Due to the connection to the canonical ensemble, fermionic Gaussian states describe ground and thermal states of quadratic Hamiltonians [8].

As explicitly shown in appendix (A.1), a fermionic Gaussian state is fully described by its covariance matrix (CM) defined as

$$\Gamma_{ab} = \frac{\mathrm{i}}{2} \mathrm{Tr} \left(\rho \left[c_a, c_b \right] \right), \quad 1 \le a, b \le 2n$$
(2.5)

which is a matrix of expectation values of quadratic Majorana operator terms. Γ is a real, antisymmetric $2n \times 2n$ matrix. The fermionic Gaussian state formalism is not restricted to a certain number of fermions. Thus, we can describe a single fermion as well as systems of more than one fermion with their corresponding CM.

We will deal with real and complex CMs throughout our whole work. Let us introduce $CM(\mathbb{R}, 2n)$ as the group of all real, skew-symmetric $2n \times 2n$ matrices and $CM(\mathbb{C}, 2n)$ as the group of all complex, skew-hermitian $2n \times 2n$ matrices.

We will only consider quadratic Hamiltonians, but one can even describe systems with Hamiltonians of higher than quadratic order in the fermionic Gaussian state formalism. If the Hamiltonian contains quadratic terms as before and if the higher order terms can be considered as perturbations on the quadratic Hamiltonian, then the ground state can be approximated by a density matrix as in (2.4). All expectation values for operators with terms that are of higher than quadratic order can be calculated using Wick's theorem [5, 6, 8].

A real, antisymmetric and even-dimensional matrix has eigenvalues that are purely imaginary or zero, which come in complex conjugated pairs. Let us call them $\pm i \cdot \lambda_j$ for Γ , $\lambda_j \in \mathbb{R}$ and j = 1, 2, ..., n. To describe a fermionic state, the CM has to satisfy the condition $i \cdot \Gamma \leq 1$, which implies $\lambda_j \in [-1, 1]$ as a condition for the eigenvalues [5, 6, 8]. In case of pure states, all λ_j have to be either 1 or -1, and for mixed states, there are eigenvalues which fulfill $|\lambda_j| < 1$. It is further known, that any real, antisymmetric and even-dimensional matrix can be brought to block-diagonal form with an orthogonal transformation O [9, p. 218]:

$$\boldsymbol{\Gamma} = \boldsymbol{O}^T \cdot \widetilde{\boldsymbol{\Gamma}} \cdot \boldsymbol{O} \quad \text{with} \quad \widetilde{\boldsymbol{\Gamma}} = \bigoplus_{j=1}^n \begin{pmatrix} 0 & \lambda_j \\ -\lambda_j & 0 \end{pmatrix}.$$
(2.6)

The Matrix H, which appears in the density matrix eq. (2.4), has block-diagonal form

$$\widetilde{\boldsymbol{H}} = \bigoplus_{j=1}^{n} \begin{pmatrix} 0 & -\beta_j \\ \beta_j & 0 \end{pmatrix}.$$
(2.7)

Then, one can show that H and Γ are brought to block-diagonal form by the same orthogonal transformation O. The eigenvalues of Γ and H are related which means that we can calculate the Hamiltonian \mathcal{H} of the system when we know its CM. This very important connection is shown in [6], the relation between the eigenvalues is given by

$$\lambda_j = \tanh\left(\frac{\beta_j}{2}\right). \tag{2.8}$$

The orthogonal transformation O can also be understood as acting on the Majorana operators in the exponent of the density matrix. They are transformed to new Majorana operators \tilde{c}_j . For these, there is a simple expression of the density matrix because of the block diagonality of the matrix \tilde{H} , namely

$$\boldsymbol{\rho} = \frac{1}{2^n} \prod_{j=1}^n \left(\mathbb{1} + \mathbf{i} \cdot \tanh\left(\frac{\beta_j}{2}\right) \cdot \widetilde{c}_{2j-1} \widetilde{c}_{2j} \right).$$
(2.9)

For a detailed calculation, please refer to Appendix A.1.

2.1.2. Jamiołkowski Isomorphism

Later, when we describe GfPEPS, we want to apply completely positive Gaussian maps [5], which are maps that transform a Gaussian state into a Gaussian state. So in general, such a map \mathcal{E} transforms a state of n fermions, described by a Γ_{in} , into a state of m fermions, described by a Γ_{out} . According to the Jamiołkowski isomorphism [3, 5, 6, 10], these maps \mathcal{E} are also described by a covariance matrix, which we call $\mathcal{G} \in CM(\mathbb{R}, 2n + 2m)$. This CM can be understood as composed of two subsystems (1 and 2 in fig. 2.1). We will call subsystem 2 the input port of \mathcal{G} and subsystem 1 the output port of \mathcal{G} . The Jamiołkowski isomorphism can be understood as projecting the 2n modes of Γ_{in} and the 2n input modes of the input port onto a maximally entangled state which will cause the output Γ_{out} to be contained in the 2m modes of the output port.

 $\boldsymbol{\mathcal{G}}$ is given by

$$oldsymbol{\mathcal{G}} = \left(egin{array}{cc} oldsymbol{A} & oldsymbol{B} \ -oldsymbol{B}^T & oldsymbol{C} \end{array}
ight), \qquad \mathrm{i}oldsymbol{\mathcal{G}} \leq \mathbb{1}$$



Figure 2.1.: Representation of the map $\mathcal{E} : \Gamma_{in} \to \Gamma_{out}$ in the Jamiołkowski isomorphism. The input state 3 and the state 2 (related to one subsystem of the state dual to the map) are projected onto a maximally entangled state (M.E., shown by the curly bracket). The output of the map is then contained in state 1. [10]

with $A \in CM(\mathbb{R}, 2m)$, $B \in \mathbb{R}^{2m \times 2n}$ and $C \in CM(\mathbb{R}, 2n)$. The resulting transformation is calculated as shown in [5] as

$$\Gamma_{\mathrm{out}} = \mathcal{E}\left(\Gamma_{\mathrm{in}}\right) = \boldsymbol{A} + \boldsymbol{B} \cdot \left(\boldsymbol{C} + \Gamma_{\mathrm{in}}^{-1}\right)^{-1} \cdot \boldsymbol{B}^{T}$$

While the map is described by a CM, just as the states themselves, we will sometimes call \mathcal{G} the state dual to the map.

2.1.3. Partial Traces for Fermionic Gaussian States

We now want to show that we can neglect the modes of a covariance matrix \mathcal{G} that are traced out in the output state. This means that the calculation of partial traces is quite simple in the fermionic Gaussian state formalism, what we will use later in our work.

Let us consider a fermionic Gaussian state with k fermionic modes (k > 1), which is described by a density matrix ρ as in eq. (2.4) and a corresponding $\Gamma \in CM(\mathbb{R}, 2k)$. We can naturally divide the system into two subsystems 1 and 2 and assign the first 2n Majorana operators to system 1 and the last 2m Majorana operators to 2 (such that n + m = k). We want to calculate the partial trace over system 2 now, resulting in a reduced density matrix of system 1, i. e. $\rho_1 = \text{Tr}_2(\rho)$. The reduced system will be a fermionic Gaussian state, as well, which is described by a

$$\Gamma_{ab}^{1} = \operatorname{Tr}_{1}(\rho_{1}[c_{a}, c_{b}]) \quad a, b = 1, \dots, 2n
= \operatorname{Tr}_{1}(\operatorname{Tr}_{2}(\rho)[c_{a}, c_{b}]) = \operatorname{Tr}_{1}(\operatorname{Tr}_{2}(\rho[c_{a}, c_{b}]))
= \operatorname{Tr}(\rho[c_{a}, c_{b}]) = \Gamma_{ab}.$$
(2.10)

We can put the $[c_a, c_b]$ into the trace over 2 because these Majorana operators only act on system 1. Therefore the $\Gamma^1 \in CM(\mathbb{R}, 2n)$ for the reduced system is just the first $2n \times 2n$ submatrix of Γ .

This has a direct consequence for the calculation of the output state of a mapping. We



Figure 2.2.: Jamiołkowski isomorphism for a map with two subsystems as an output of which one is traced out in the end.

consider a map now, that transforms an input state of arbitrary many fermions to an output state of k = n + m fermions. As before, we can naturally divide the output into two subsystems of which one will be traced out in the end. This is, the output port of the CM that describes the map can be interpreted as consisting of two subsystems 1 and 2 (see fig. 2.2). This is the only difference to the general case which we discussed in the previous section. Therefore, such a map is described by

$$oldsymbol{\mathcal{G}} = \left(egin{array}{cccc} oldsymbol{A}_1 & oldsymbol{A}_{12} & oldsymbol{B}_1 \ -oldsymbol{A}_{12}^T & oldsymbol{A}_2 & oldsymbol{B}_2 \ -oldsymbol{B}_1^T & -oldsymbol{B}_2^T & oldsymbol{C} \end{array}
ight)$$

which acts on an input state Γ_{in} . According to the Jamiołkowski isomorphism, the resulting output is calculated as

$$m{\Gamma}_{ ext{out}} = egin{pmatrix} m{A}_1 & m{A}_{12} \ -m{A}_{12}^T & m{A}_2 \end{pmatrix} + egin{pmatrix} m{B}_1 \ m{B}_2 \end{pmatrix} \cdot ig(m{C} + m{\Gamma}_{ ext{in}}^{-1}ig)^{-1} \cdot ig(m{B}_1^T & m{B}_2^Tig).$$

We will now trace out system 2 in the output and due to eq. (2.10), the CM of the reduced state is given by

$$\Gamma_{\text{out}}^1 = \boldsymbol{A}_1 + \boldsymbol{B}_1 \cdot \left(\boldsymbol{C} + \Gamma_{\text{in}}^{-1}\right)^{-1} \cdot \boldsymbol{B}_1^T.$$

But this is just the same Jamiołkowski formula as for a map that transforms the input state to only the output state of system 1, where the map is described by a CM

$$\mathcal{G}' = \left(egin{array}{cc} m{A}_1 & m{B}_1 \ -m{B}_1^T & m{C} \end{array}
ight).$$

Or differently speaking, we can neglect the system 2 (the one that is traced out) in the CM \mathcal{G} right from the start.

2.2. Gaussian Fermionic PEPS

2.2.1. PEPS for Spin Systems

Projected Entangled Pair States (PEPS) are expected to give good approximations to ground and thermal states of spin systems with local Hamiltonians due to the area law [3, 6, 11]. We want to give a brief overview of the construction of PEPS, while the construction of Gaussian fermionic PEPS is a very similar PEPS construction for fermionic Gaussian states.



Figure 2.3.: Construction of a two-dimensional PEPS for spin systems. The auxiliary states each have dimension D and the projections map from the 4D dimensional subsystem to the d dimensional physical state. (Figure similar to [11])

Given spins on a square lattice in two spatial dimensions, PEPS are constructed by assigning four auxiliary *D*-dimensional modes to each physical site. Each of these auxiliary modes is in a maximally entangled state $|\omega\rangle = \sum_{i=1}^{D} |i, i\rangle$ with an auxiliary mode from the neighboring physical site. We apply a linear map at each site, which maps the auxiliary system to the physical one (see fig. 2.3).

2.2.2. Gaussian Fermionic PEPS on a Cylinder

In order to describe two-dimensional systems of fermionic Gaussian states, we have to adapt the PEPS construction. This ensures that the resulting state obeys fermionic anti-commutation relations and parity conservation [11]. We will call these states Gaussian fermionic PEPS (GfPEPS) and they are constructed using four auxiliary fermionic modes (α , β , γ and δ) per physical site, each of which forms a maximally entangled fermionic Gaussian state with an auxiliary fermionic mode of each neighboring site. The projection from the auxiliary system to the physical one (mode c) has to be a completely positive Gaussian map as in chapter 2.1.2, in order to map from a fermionic Gaussian auxiliary state to a fermionic Gaussian physical state. The maximally entangled state and the map are described by their corresponding CMs and the output state is calculated using Jamiołkowski's isomorphism. We will consider a translational invariant GfPEPS on a square lattice, with N_v physical sites in vertical direction and N_h physical sites in horizontal direction. We choose to have periodic boundary conditions (PBC) in vertical direction and open boundary conditions (OBC) horizontally, leading to a cylindrical GfPEPS (fig. 2.4).



Figure 2.4.: Construction of a cylindrical GfPEPS with $N_v \times N_h$ sites. Each site (apart from the boundary sites) contains four auxiliary modes and one physical mode (black dots and green dot in the enlarged site, respectively). The input state $\Gamma_{\rm in}$ contains all maximally entangled states between adjacent sites and the output state $\Gamma_{\rm out}$ can be calculated with Jamiołkowski's isomorphism and will contain all physical modes.

For this setting, we want to calculate the resulting state Γ_{out} of the system. Since the mapping from the auxiliary to the physical system is described by a CM, as well as the maximally entangled states, one can calculate Γ_{out} in different steps. Therefore, we start by calculating the CM of one maximally entangled state. Then, we take all horizontal maximally entangled states of one column as our input state and with the corresponding \mathcal{G} s of this column, we calculate the resulting output. We call this a vertical GfPEPS ring which represents N_v physical modes and the $2N_v$ horizontal auxiliary modes. This calculation is conveniently done in Fourier space due to the translation invariance of the system. We can then calculate the whole GfPEPS by combining these rings, where we have to be careful to assign the maximally entangled state to auxiliary particles with the same vertical index.

We begin by calculating $\boldsymbol{\omega} \in CM(\mathbb{R}, 4)$ for the maximally entangled state. According to [6], one can use any maximally entangled state for the bonds, as they can be locally transformed into each other and these local transformations can be absorbed in the definition of the local projectors. So we decide to take $|\varphi_{\omega}\rangle = \frac{1}{\sqrt{2}} \left(a_1^{\dagger} - ia_2^{\dagger}\right)|0\rangle$ as the maximally entangled state, where a_1^{\dagger} creates an auxiliary fermion on one site and a_2^{\dagger} creates an auxiliary fermion on the other site. We choose the same maximally entangled state for the horizontal and vertical bonds. This means for the horizontal bond that a_1^{\dagger} creates a right auxiliary fermion on site k and a_2^{\dagger} creates a left auxiliary fermion on site k + 1, and similar for the vertical bond. So, its CM can be calculated with $\omega_{ab} = \frac{i}{2} \text{Tr} \left(|\varphi_{\omega}\rangle \langle \varphi_{\omega}| [c_a, c_b] \right)$ and is

$$\boldsymbol{\omega} = \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix} \tag{2.11}$$

where c_a and c_b are out of the set of the four auxiliary Majorana operators of the corresponding maximally entangled state. This $\boldsymbol{\omega}$ is a pure state, as its eigenvalues are clearly all $\pm i$ and



Figure 2.5.: GfPEPS ring with $N_v \times 1$ sites. Only the vertical auxiliary modes are contracted. The Jamiołkowski isomorphism gives an output, which contains the physical modes as well as the two horizontal virtual modes per site.

therefore its inverse is $-\boldsymbol{\omega}$.

Then, we construct one vertical ring of the GfPEPS cylinder (fig. 2.5) and calculate its resulting state. The input state is the combination of all maximally entangled states between the vertical auxiliary modes, described by $\Omega_v \in CM(\mathbb{R}, 4N_v)$ and the resulting output is $\Gamma_{\text{out}} \in CM(\mathbb{R}, (2+4)N_v)$. It describes the N_v physical states and the 2 horizontal auxiliary states per site, i.e. $2N_v$ virtual modes in total. Hence, the state which is dual to the map is given by

$$oldsymbol{\mathcal{G}} = \left(egin{array}{cc} oldsymbol{A} & oldsymbol{B} \ -oldsymbol{B}^T & oldsymbol{C} \end{array}
ight)$$

with $\mathbf{A} \in CM(\mathbb{R}, 6N_v)$, \mathbf{B} a real $6N_v \times 4N_V$ matrix and $\mathbf{C} \in CM(\mathbb{R}, 4N_v)$. As the maximally entangled states "live" on two adjacent sites, $\mathbf{\Omega}_v$ is a circulant matrix of the form

$$m{\Omega}_v = \left(egin{array}{ccccccccc} 0 & m{\omega}_1 & 0 & 0 & \dots & m{\omega}_{-1} \ m{\omega}_{-1} & 0 & m{\omega}_1 & 0 & \dots & 0 \ 0 & m{\omega}_{-1} & 0 & m{\omega}_1 & \dots & 0 \ dots & do$$

with

$$\boldsymbol{\omega}_1 = \left(egin{array}{cc} 0 & 0 \\ \mathbbm{1} & 0 \end{array}
ight) \quad ext{and} \quad \boldsymbol{\omega}_{-1} = \left(egin{array}{cc} 0 & -\mathbbm{1} \\ 0 & 0 \end{array}
ight)$$

As we are dealing with a translational invariant system with PBC, it is convenient to switch to Fourier space representation. The Fourier transformation only acts on the block structure of the matrices. We choose the matrices \mathcal{F} that represent the Fourier transformation to be defined by $\mathcal{F}_{kl} := \frac{1}{\sqrt{N_v}} e^{-i\frac{2\pi}{N_v}kl}$ and as we encounter two different relevant block sizes, we define a $\mathcal{F}_4 := \mathcal{F} \otimes \mathbb{1}_4$ and a $\mathcal{F}_6 := \mathcal{F} \otimes \mathbb{1}_6$. This yields the Fourier transform of the output state

$$\begin{split} \hat{\boldsymbol{\Gamma}}_{\text{out}}\left(\phi_{k}\right) &= \boldsymbol{\mathcal{F}}_{6} \cdot \boldsymbol{\Gamma}_{\text{out}} \cdot \boldsymbol{\mathcal{F}}_{6}^{\dagger} = \boldsymbol{\mathcal{F}}_{6} \cdot \boldsymbol{A} \cdot \boldsymbol{\mathcal{F}}_{6}^{\dagger} + \boldsymbol{\mathcal{F}}_{6} \cdot \boldsymbol{B} \cdot \left[\boldsymbol{C} - \boldsymbol{\Omega}\right]^{-1} \cdot \boldsymbol{B}^{T} \cdot \boldsymbol{\mathcal{F}}_{6}^{\dagger} \\ &= \boldsymbol{\mathcal{F}}_{6} \cdot \boldsymbol{A} \cdot \boldsymbol{\mathcal{F}}_{6}^{\dagger} + \boldsymbol{\mathcal{F}}_{6} \cdot \boldsymbol{B} \cdot \boldsymbol{\mathcal{F}}_{4}^{\dagger} \left[\boldsymbol{\mathcal{F}}_{4} \cdot \boldsymbol{C} \cdot \boldsymbol{\mathcal{F}}_{4}^{\dagger} - \boldsymbol{\mathcal{F}}_{4} \cdot \boldsymbol{\Omega} \cdot \boldsymbol{\mathcal{F}}_{4}^{\dagger}\right]^{-1} \boldsymbol{\mathcal{F}}_{4} \cdot \boldsymbol{B}^{T} \cdot \boldsymbol{\mathcal{F}}_{6}^{\dagger} \\ &= \boldsymbol{A} + \boldsymbol{B} \left[\boldsymbol{C} - \hat{\boldsymbol{\Omega}}_{v}\left(\phi_{k}\right)\right]^{-1} \boldsymbol{B}^{T}. \end{split}$$

Here, we have used the property $\mathcal{F}_4^{\dagger} \cdot \mathcal{F}_4 = \mathbb{1}$ and the invariance of the matrices A, B and C under the chosen Fourier transformation, due to their block diagonal form. As Ω_v is a circulant matrix, its Fourier transformed $\hat{\Omega}_v$ is a block diagonal matrix

$$\hat{\mathbf{\Omega}}_{v} = \bigoplus_{k=0}^{N_{v}-1} \left(\begin{array}{cc} 0 & -\mathrm{e}^{-\mathrm{i}\phi_{k}} \cdot \mathbb{1} \\ \mathrm{e}^{\mathrm{i}\phi_{k}} \cdot \mathbb{1} & 0 \end{array} \right),$$

with $\phi_k = \frac{2\pi k}{N_v}$. We can thus fully describe the problem by a $\hat{\Gamma}_{out}(\phi_k) \in CM(\mathbb{C}, 6)$ depending on an angle ϕ_k (we will suppress the index k from now on).

We can now go on and "grow" our GfPEPS further, for which the input is composed of the N_v horizontal maximally entangled states, expressed by

$$oldsymbol{\Omega}_h = igoplus_{k=1}^{N_v} oldsymbol{\omega}$$

We have to be careful that we put the maximally entangled states between two auxiliary particles of both rings with the same vertical index. Ω_h is a block-diagonal matrix and hence invariant under the previously introduced Fourier transformation \mathcal{F}_4 . Thus, we can do the growth in Fourier space. Therefore, we take two $\hat{\Gamma}_{out}$ from before and combine them together to form a new \mathcal{G} . We have to take two $\hat{\Gamma}_{out}$ of the same angle ϕ to combine the rings properly. We also have to be careful and reorder the entries as the input channel of \mathcal{G} consists of one mode of the first $\hat{\Gamma}_{out,L}$ and one mode of the second $\hat{\Gamma}_{out,R}$ (fig. 2.6). After applying the Jamiołkowski isomorphism, we will get a new $\hat{\Gamma}_{out}(\phi)$ that contains two auxiliary modes as before but also two physical modes.

This procedure can either be applied iteratively, which means that we always add one ring to the new $\hat{\Gamma}_{out}$, or recursively, where we combine two new $\hat{\Gamma}_{out}$ and apply Jamiołkowski's isomorphism (or a combination of both) until we have a GfPEPS of $N_v \times (N_h - 2)$ sites. Then, we have to add the boundary rings, which have a physical mode and only one horizontal auxiliary mode per site. The procedure of combining them with the previously obtained $\hat{\Gamma}_{out}$ is basically the same. This means that all auxiliary modes are part of the input port of \mathcal{G} and that the output port only contains physical modes. Hence, the resulting output after this step only contains physical modes and represents the physical system.



Figure 2.6.: Combine two $\hat{\Gamma}_{out}$ to a new \mathcal{G} and apply Jamiołkowski's isomorphism.

In the end, we are interested in Γ_{out} in real space, which we can calculate by taking the inverse Fourier transformation of $\hat{\Gamma}_{\text{out}}(\phi)$.

In the next chapters, we will consider reduced GfPEPS and we will be interested in the state of only the auxiliary system. The calculation of the auxiliary system can be done straightforwardly, we just have to neglect the physical modes in the CM that describes the map.

3. Entanglement spectra and boundary theories

All PEPS satisfy the so called area law and there is consistently a close relation between the entanglement spectrum and the boundary of a system [1, 12].

On a cylinder, we can naturally divide the PEPS in a left and a right part. If we trace out the right part of the PEPS, we get a reduced density matrix for the left part. We can assign a Hamiltonian to that reduced density matrix with $\rho_L \propto \exp(-\beta H)$. The entanglement spectrum is defined as the spectrum of this Hamiltonian. It contains information about the whole system and is described by a one dimensional theory, for certain systems [1]. Although the whole system is a two dimensional one, this one dimensionality in the entanglement spectrum seems to reflect the area law, which means that all the relevant physics between two regions of a system happens at the boundary of the regions (rather than in the whole volume). For PEPS, this one dimensionality has a very illustrative character. One can show that the entanglement spectrum is directly related to the spectrum of the virtual particles at the boundary. We want to give a brief overview of this relation for PEPS, before we want to show here that the entanglement spectrum for GfPEPS is also directly connected to the auxiliary states at the boundary.

3.1. Entanglement spectrum for PEPS

In [1], the relation for the reduced density matrix of a PEPS of fermionic spins on a cylinder and its reduced density matrices for the auxiliary system are derived. We consider a PEPS of dimension $N_v \times N_h$ and divide it in a left part, containing the first *l* columns, and a right part, containing the remaining $N_h - l$ columns. Its reduced density matrix ρ_L is calculated by tracing out the physical states of the right side. The reduced density matrices for the auxiliary systems σ_L and σ_R are calculated by contracting all auxiliary and physical indices but the auxiliary indices between the *l*-th and (l + 1)-th column of the left/right part of the PEPS. It can be shown that the reduced density matrix is given by

$$oldsymbol{
ho}_L = oldsymbol{U} \sqrt{oldsymbol{\sigma}_L^T} oldsymbol{\sigma}_R \sqrt{oldsymbol{\sigma}_L^T} oldsymbol{U}^\dagger$$

with an isometry U mapping from the auxiliary to the physical system. As already introduced in the previous section, we can assign a Hamiltonian to the reduced density matrix with $\rho_L = \exp(-\beta H)/Z$. Similarly, we can assign Hamiltonians to the density matrices of the auxiliary



Figure 3.1.: GfPEPS of the reduced state. The red dots describe sites, where there are only the four (or three) auxiliary particles left after tracing out the physical particle. The black dots contain four (three) auxiliary and one physical particle, as before in the GfPEPS construction.

systems, σ_L and σ_R . The isometry U has no influence on the spectrum and consequently, the spectrum of ρ_L is directly related to the spectrum of the reduced density operators σ_L and σ_R of the virtual subsystem.

For some systems with appropriate symmetries, it is $\boldsymbol{\sigma}_L^T = \boldsymbol{\sigma}_R$ and thus the spectrum of $\boldsymbol{\sigma}_R^2 = \frac{1}{Z^2} \exp(-2\beta \boldsymbol{H}_R)$ is directly connected to the spectrum of $\boldsymbol{\rho}_L$.

3.2. Entanglement spectrum for GfPEPS

We want to calculate the relation between the entanglement spectrum and the boundary for a GfPEPS on a cylinder of dimension $N_v \times N_h$. The left part of the GfPEPS contains $N_v \times l$ physical sites which are described by the first $2n = 2 \cdot N_v \cdot l$ Majorana operators. The right part contains $N_v \times (N_h - l)$ sites, described by the last $2m = 2 \cdot N_v \cdot (N_h - l)$ Majorana operators. Both sides are connected via the N_v maximally entangled states of the auxiliary system.

The reduced density matrix ρ_L can be calculated by taking the partial trace over the right side of the system, as shown in section 2.1.3. The reduced system is described by a $\Gamma_L \in CM(\mathbb{R}, 2n)$ which is the (1, 1)-block of the CM Γ of the complete GfPEPS. As also shown in section 2.1.3, we can omit the physical states in the right side of the GfPEPS from the beginning (see fig. 3.1). The left and right part can be calculated independently as described in section 2.2.2. The resulting CM describing the left part is represented by the $2 \cdot N_v \cdot l$ Majorana operators for the physical sites and the $2 \cdot N_v$ Majorana Operators of the virtual subsystem. The CM for the right side is fully described by the $2 \cdot N_v$ Majorana operators for the auxiliary modes.

As before, it is suitable to describe the system in Fourier space. Thus, the left part is given by a

$$\hat{m{\Gamma}}_L = \left(egin{array}{cc} \hat{m{A}}_L & \hat{m{B}}_L \ - \hat{m{B}}_L^\dagger & \hat{m{C}}_L \end{array}
ight)$$

with $\hat{A}_L \in CM(\mathbb{C}, 2l+2), B \in \mathbb{C}^{(2l+2) \times 2}$ and $\hat{C}_L \in CM(\mathbb{C}, 2)$ which all depend implicitly on an



Figure 3.2.: Sketch for the tracing out of one mode in the GfPEPS construction.

angle ϕ (see sec. 2.2.2). To describe the right half, we do not have to include a physical system. Hence, $\hat{C}_R \in CM(\mathbb{C}, 2)$ also depends on the angle ϕ and we can construct the CM corresponding to the map with these two CMs and it is given by

$$\hat{\boldsymbol{\mathcal{G}}} = \left(egin{array}{ccc} \hat{\boldsymbol{A}}_L & \hat{\boldsymbol{B}}_L & 0 \ -\hat{\boldsymbol{B}}_L^\dagger & \hat{\boldsymbol{C}}_L & 0 \ 0 & 0 & \hat{\boldsymbol{C}}_R \end{array}
ight).$$

The maximally entangled state, which is the input for the Jamiołkowski isomorphism, is given by

$$\boldsymbol{\omega} = \left(\begin{array}{cc} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{array}\right),$$

which, together with $\boldsymbol{\mathcal{G}}$, gives an output state

$$\hat{\boldsymbol{\Gamma}}_{\text{out},L} = \hat{\boldsymbol{A}}_{L} + \begin{pmatrix} \hat{\boldsymbol{B}}_{L} \\ 0 \end{pmatrix} \cdot \begin{pmatrix} \hat{\boldsymbol{C}}_{L} & -\mathbb{1} \\ \mathbb{1} & \hat{\boldsymbol{C}}_{R} \end{pmatrix}^{-1} \cdot \begin{pmatrix} \hat{\boldsymbol{B}}_{L}^{\dagger} & 0 \end{pmatrix}$$

$$= \hat{\boldsymbol{A}}_{L} + \hat{\boldsymbol{B}}_{L} \cdot \left(\hat{\boldsymbol{C}}_{L} + \hat{\boldsymbol{C}}_{R}^{-1} \right)^{-1} \cdot \hat{\boldsymbol{B}}_{L}^{\dagger}$$
(3.1)

where we have used the formula for the inverse of a block matrix as in [13, p. 472]. The combination of both sides is sketched in fig. 3.2. As one can see from eq. (3.1), this is the Jamiołkowski isomorphism for a map that is described by a CM $\hat{\Gamma}_L$ acting on an input state \hat{C}_R . This is clear, because we projected \hat{C}_L and one side of the maximally entangled input onto a maximally entangled state and \hat{C}_R and the other side of the maximally entangled input onto another maximally entangled state. This is the same as projecting the two \hat{C}_S onto a maximally entangled state, directly.

Applying the inverse Fourier transform leads to an expression in real space, which yields

$$\boldsymbol{\Gamma}_{ ext{out},L} = \boldsymbol{A}_L + \boldsymbol{B}_L \cdot \left(\boldsymbol{C}_L + \boldsymbol{C}_R^{-1} \right)^{-1} \cdot \boldsymbol{B}_L^T.$$

This expression shows that the entanglement spectrum of the reduced density matrix for GfPEPS not only depends on physical and auxiliary Majorana operators of the left subsystem but also on the auxiliary Majorana operators of the right subsystem. C_L and C_R describe the auxiliary systems for GfPEPS like the σ_L and σ_R do for PEPS.

To show that the spectrum of the auxiliary system is the same as the spectrum of the reduced GfPEPS, we have to transform the $\Gamma_{\text{out},L}$ to get a CM that is only dependent on C_L and C_R . We want to use the freedom in purifications from [14, p. 110f.] to get an $\Gamma'_{\text{out},L}$ that is the same as the $\Gamma_{\text{out},L}$ up to an orthogonal transformation.

As mentioned before, one can think of the C_R as the input state and

$$oldsymbol{\mathcal{G}} = \left(egin{array}{cc} oldsymbol{A}_L & oldsymbol{B}_L \ -oldsymbol{B}_L^\dagger & oldsymbol{C}_L \end{array}
ight)$$

as the CM that describes the map in the Jamiołkowski isomorphism. Let us consider a \mathcal{G} that transforms a pure input state to a pure output state, i.e. $-\mathcal{G}^2 = \mathbb{1}$. We can think of \mathcal{G} as composed of two subsystems, 1 and 2. So A_L is the CM describing subsystem 1 and C_L describes subsystem 2. B_L is a term connecting both subsystems. When we trace out system 1 in \mathcal{G} , we only get C_L .

Let us consider another pure \mathcal{G}' , which describes two subsystems. We want \mathcal{G}' to have the same (2, 2)-block as \mathcal{G} , i. e. C_L . This means that the reduced state after tracing out system 1 is also described by C_L , as before. Then, the aforementioned freedom in purification tells us that \mathcal{G}' is connected to \mathcal{G} via an orthogonal transformation of subsystem 1, i. e.

$$\mathcal{G}' = \left(egin{array}{cc} \mathbf{O} & 0 \\ 0 & 1 \end{array}
ight) \cdot \mathcal{G} \cdot \left(egin{array}{cc} \mathbf{O}^T & 0 \\ 0 & 1 \end{array}
ight).$$

If we calculate the Jamiołkowski isomorphism with this \mathcal{G}' we get a

$$\Gamma'_{\mathrm{out},L} = \boldsymbol{O} \cdot \boldsymbol{\Gamma}_{\mathrm{out},L} \cdot \boldsymbol{O}^T$$

what we wanted to find.

We choose a

$$\mathcal{G}' = \left(egin{array}{ccc} -m{C}_L & \sqrt{m{C}_L^2 + \mathbb{1}} \ -\sqrt{m{C}_L^2 + \mathbb{1}} & m{C}_L \end{array}
ight)$$

which satisfies all conditions from before and thus we get a $\Gamma'_{\text{out},L}$ which is the same as $\Gamma_{\text{out},L}$ up to an orthogonal transformation,

$$\boldsymbol{O} \cdot \boldsymbol{\Gamma}_{\text{out},L} \cdot \boldsymbol{O}^{T} = \boldsymbol{\Gamma}_{\text{out},L}^{\prime} = -\boldsymbol{C}_{L} + \sqrt{\boldsymbol{C}_{L}^{2} + \mathbb{1}} \cdot \left(\boldsymbol{C}_{L} + \boldsymbol{C}_{R}^{-1}\right)^{-1} \cdot \sqrt{\boldsymbol{C}_{L}^{2} + \mathbb{1}}.$$
(3.2)

Similar to the PEPS case, the entanglement spectrum is the same as the spectrum of $\Gamma'_{out L}$.

As mentioned in the previous section, a symmetry yielding $\boldsymbol{\sigma}_L^T = \boldsymbol{\sigma}_R$ for PEPS means that the entanglement spectrum of $\boldsymbol{\rho}_L$ is connected to the spectrum of $\boldsymbol{\sigma}_R^2$. Hence, the inverse temperature β connected to $\boldsymbol{\rho}_L$ is twice the inverse temperature of $\boldsymbol{\sigma}_R$. We want to see, if there is a symmetry in the GfPEPS case that yields to the same relation. We can connect the eigenvalues of \boldsymbol{C}_R to an inverse temperature with the relation $i \cdot \lambda_j = i \cdot \tanh\left(\frac{\beta_j}{2}\right)$. Hence, we want to find a $\Gamma'_{\text{out},L}$ which has a temperature $\beta'_j = 2\beta_j$. This is then connected to the eigenvalues of $\Gamma'_{\text{out},L}$ via

$$\mathbf{i} \cdot \lambda_j' = \mathbf{i} \cdot \tanh(\beta_j) = \mathbf{i} \cdot \tanh(2 \cdot \operatorname{artanh}(\lambda_j)) = \frac{2\mathbf{i} \cdot \lambda_j}{1 - (\mathbf{i} \cdot \lambda_j)^2}$$

This relation for the eigenvalues can be generalized to a matrix relation, namely

$$\Gamma_{\text{out},L}' = \frac{2C_R}{\mathbb{1} - C_R^2}.$$
(3.3)

The matrix in the denominator describes the matrix inverse. So, if we can find a symmetry that leads to this relation, we expect the spectrum of the reduced state to have an inverse temperature that is twice the inverse temperature of the auxiliary subsystem. One can easily check by inserting $C_R = -C_L$ in eq. (3.2) that this leads to such a case. Thus, we can conclude that the chosen symmetry which leads to $C_R = -C_L$ is the same as in the PEPS construction for $\sigma_L^T = \sigma_R$.

We have seen that the entanglement spectrum of the reduced state ρ_L has a strong dependence on the spectrum of the reduced auxiliary system. For certain symmetries, there is even a direct connection between both spectra. One can deduce the properties of the entanglement spectrum from the boundary spectrum of the auxiliary particles and their corresponding Hamiltonians, so it is very enlightening to investigate those. The discussion in the next chapters will focus on that.

4. Analytically provable properties for GfPEPS

As we have seen in the previous chapters, it is very enlightening to investigate the reduced state of the auxiliary system of the GfPEPS. In this chapter, we want to construct this reduced auxiliary state and show some properties for it. As it is very hard to calculate the resulting auxiliary state analytically, we only can calculate these properties for special cases.

First, we want to consider a system whose CM corresponding to the map has only non-zero entries for combinations of only even or only odd Majorana operators. For such a system, we can show for all but one special case that the off-diagonal terms in the resulting CM are exponentially decaying with the number of sites in horizontal direction. This means that the two boundaries decompose.

Then, we want to go back to more general systems, where there are no zero entries from the beginning. Here, we will show the decay of the off-diagonal terms for certain cases, as well.

We showed in section 2.2.2, how to construct GfPEPS. Here, we do a straightforward construction for the auxiliary subsystem of the GfPEPS, which we want to show again briefly. In general, we calculate the resulting CM for a cylindrical system that only consists of virtual particles (see fig. 4.1). This is the reduced state of the auxiliary system which is connected to the reduced density matrix of the GfPEPS, as shown in chapter 3.2. The input state in the construction of the system is the combination of all maximally entangled states $|\varphi_{\omega}\rangle = \frac{1}{\sqrt{2}} (\alpha_1 - i \cdot \alpha_2) |0\rangle$ between all adjacent sites. The state dual to the map is described in general by an $8 \cdot N_v \cdot N_h \times 8 \cdot N_v \cdot N_h$



Figure 4.1.: System of only auxiliary particles, which is connected to the reduced density matrix. The resulting CM has the virtual particles of the left and right boundary as an output.

dimensional, block-diagonal covariance matrix. Due to translational invariance, it is fully described by an 8×8 covariance matrix, containing the expectation values of quadratic Majorana operators of the four virtual particles of one site. Here, we want to do the calculation for a cylinder, which has $2N_v$ auxiliary modes as an output on each side. So in contrast to the Gf-PEPS construction in chapter 2.2.2, we do not add a boundary ring which contracts all auxiliary particles on one side. Hence, the resulting state is described by a $4N_v \times 4N_v$ matrix Γ_{out} . This calculation is done as in chapter 2.2.2, which means that we construct rings in Fourier space and combine these rings to the full system.

4.1. Models with non-interacting Majorana operators c_{2i-1} and c_{2j}

As mentioned before, it is very hard to calculate the CM of an auxiliary system analytically. Therefore, we want to discuss a special case first, for which we can give analytical results. We consider a system of virtual particles whose map is described at each site by a real, antisymmetric CM of the form

$$\boldsymbol{\mathcal{G}} = \begin{pmatrix} 0 & 0 & a_1 & 0 & b_1 & 0 & c_1 & 0 \\ 0 & 0 & 0 & a_2 & 0 & b_2 & 0 & c_2 \\ -a_1 & 0 & 0 & 0 & d_1 & 0 & e_1 & 0 \\ 0 & -a_2 & 0 & 0 & 0 & d_2 & 0 & e_2 \\ -b_1 & 0 & -d_1 & 0 & 0 & 0 & f_1 & 0 \\ 0 & -b_2 & 0 & -d_2 & 0 & 0 & 0 & f_2 \\ -c_1 & 0 & -e_1 & 0 & -f_1 & 0 & 0 & 0 \\ 0 & -c_2 & 0 & -e_2 & 0 & -f_2 & 0 & 0 \end{pmatrix}$$

This means, that all entries of the CM that combine an even and odd Majorana operator are zero. We can rearrange \mathcal{G} by choosing a different sorting of the Majorana operators: $\{\alpha_1, \beta_1, \gamma_1, \delta_1, \alpha_2, \beta_2, \gamma_2, \delta_2\}$. Then, we get a block-diagonal matrix $\mathcal{G} = \mathcal{G}^{(1)} \oplus \mathcal{G}^{(2)}$ with

$$\boldsymbol{\mathcal{G}}^{(i)} = \begin{pmatrix} 0 & a_i & b_i & c_i \\ -a_i & 0 & d_i & e_i \\ -b_i & -d_i & 0 & f_i \\ -c_i & -e_i & -f_i & 0 \end{pmatrix}, \quad i = 1, 2.$$

These two blocks never couple in the calculation of the output state of the complete auxiliary system. Hence, we can calculate the output for the even and odd Majorana operators independently. This is, we can do the calculations similar to chapter 2.2.2, but with all occurring CMs of half the size compared to the original ones. We will omit the dependence on (i) in the following discussion.

After the Fourier-Transform and the application of the Jamiołkowski isomorphism, we will have a CM $\hat{\Gamma}_0$, which is a 2 × 2 skew-hermitian matrix, depending on an angle ϕ . This $\hat{\Gamma}_0$ describes one vertical ring of the auxiliary system. Similar to chapter 2.2.2, we can combine



Figure 4.2.: Sketch for the recursive (a) and iterative (b) application of the Jamiołkowski isomorphism. In (a), the *n*-th CM Γ_n describes 2^n vertical rings. In (b), the *k*-th Γ_k describes k + 1 vertical rings.

the system either recursively or iteratively to get the CM of the complete auxiliary system, see fig. 4.2. Applying the Jamiołkowski isomorphism will map Gaussian states onto Gaussian states again, so the general form of the CM will stay the same and after applying the isomorphism ktimes, we find

$$\hat{\boldsymbol{\Gamma}}_{k} = \begin{pmatrix} ia_{k}(\phi) & b_{k}(\phi) \\ -\bar{b}_{k}(\phi) & ic_{k}(\phi) \end{pmatrix}, \quad k = 0, \dots, N_{v}$$

$$(4.1)$$

where $a_k(\phi), c_k(\phi) \in \mathbb{R}$ and $b_k(\phi) \in \mathbb{C}$. In the following, we will suppress the angle ϕ .

We know that all eigenvalues of a skew-hermitian matrix are imaginary and from the condition $\hat{\mathbf{\Gamma}}_0 \leq \mathbb{1}$ that all eigenvalues of $\hat{\mathbf{\Gamma}}_0$ have to be between -1 and 1. Since the Jamiołkowski isomorphism maps Gaussian states onto Gaussian states, this condition holds for all $\hat{\mathbf{\Gamma}}_k$. The eigenvalues of $\hat{\mathbf{\Gamma}}_k$ are

$$-1 \leq \frac{1}{2} \left(a_k + c_k \pm \sqrt{(a_k - c_k)^2 + 4 \cdot |b_k|^2} \right) \leq 1$$

$$\Leftrightarrow \quad 0 \leq |a_k + c_k| \leq 2 - \sqrt{(a_k - c_k)^2 + 4 \cdot |b_k|^2} \leq 2 - 2 \cdot |b_k|$$
(4.2)

One can see from these formulas that

$$a_k, c_k \in [-1, 1] \text{ and } |b_k| \in [0, 1].$$
 (4.3)

4.1.1. Recursive application of the Jamiołkowski isomorphism

In this section, we want to calculate the state of the auxiliary particles by recursively applying Jamiołkowski's isomorphism, see fig. 4.2(a). We call the output state after n recursive applications $\hat{\Gamma}_n$. Hence, it will describe a system consisting of 2^n vertical rings. We do not consider a certain number of sites in horizontal direction, as we want to show that the off-diagonal terms

in $\hat{\Gamma}_n$ tend to zero for large systems. We do this by deriving recurrence formulas for the entries of the covariance matrix $\hat{\Gamma}_n$ and show that the off-diagonal term vanishes.

We start with two rings, each described by $\hat{\Gamma}_0$. These two rings can be combined to a \mathcal{G} that describes the map from a maximally entangled state $\boldsymbol{\omega}$ to $\hat{\Gamma}_1$. The input state for the Jamiołkowski isomorphism is given by

$$\boldsymbol{\omega} = \left(\begin{array}{cc} 0 & 1\\ -1 & 0 \end{array}\right).$$

The resulting state is described by $\hat{\Gamma}_1$. We then combine two $\hat{\Gamma}_1$ s to get a $\hat{\Gamma}_2$ and so on.

So in each step we group two $\hat{\Gamma}_n$ together (where we have to choose the ordering as $\{\alpha_L, \beta_R, \beta_L, \alpha_R\}$ similar to fig. 2.6) and get a state dual to the map

$${\cal G} = \left(egin{array}{ccccc} {
m i}a_n & 0 & b_n & 0 \ 0 & {
m i}c_n & 0 & -ar b_n \ -ar b_n & 0 & {
m i}c_n & 0 \ 0 & b_n & 0 & {
m i}a_n \end{array}
ight).$$

Applying Jamiołkowski's isomorphism, yields

$$\hat{\mathbf{\Gamma}}_{n+1} = \begin{pmatrix} \mathbf{i}a_n & 0\\ 0 & \mathbf{i}c_n \end{pmatrix} + \frac{1}{1 - a_n \cdot c_n} \begin{pmatrix} \mathbf{i} \cdot a_n \cdot |b_n|^2 & -b_n^2\\ \bar{b}_n^2 & \mathbf{i} \cdot c_n \cdot |b_n|^2 \end{pmatrix}.$$

This means that the new entries of $\ddot{\Gamma}_{n+1}$ can be calculated with the entries of $\ddot{\Gamma}_n$. This yields recurrence formulas for the entries

$$a_{n+1} = a_n + a_n \cdot \frac{|b_n|^2}{1 - a_n \cdot c_n} = a_n \cdot (1 + \lambda_n)$$
(4.4)

$$c_{n+1} = c_n + c_n \cdot \frac{|b_n|^2}{1 - a_n \cdot c_n} = c_n \cdot (1 + \lambda_n)$$
(4.5)

$$b_{n+1} = -\frac{b_n^2}{1 - a_n \cdot c_n} = -\frac{b_n}{\bar{b}_n} \cdot \frac{|b_n|^2}{1 - a_n \cdot c_n} = -\frac{b_n}{\bar{b}_n} \cdot \lambda_n$$
(4.6)

where we have defined the λ_n as

$$\lambda_n = \frac{|b_n|^2}{1 - a_n \cdot c_n}.\tag{4.7}$$

Starting from the recurrence formulas (4.4)-(4.6) and eq. (4.7), we can derive a recurrence formula for λ which contains λ_{n-1} , λ_n and λ_{n+1} :

$$\lambda_{n+1} = \frac{\lambda_n^3}{\lambda_{n-1}^2 \cdot (1+\lambda_n)^2 - 2 \cdot \lambda_n^2 - \lambda_n^3}.$$
(4.8)

We want to show now that the λ_n tend to zero for increasing n, for all but one starting CM.

To this end, we have to show that the λ_n are bounded and strictly monotone decreasing for increasing n. Then, there exists a limit which is approached for infinitely large n. The λ_n is directly related to the off-diagonal entry b_{n+1} of $\hat{\Gamma}_{n+1}$. This off-diagonal term is the expectation value of $\alpha \cdot \beta$, where α is a Majorana operator of a virtual particle on the left boundary and β for a virtual particle on the right boundary. As λ_n tends to zero for large systems, the expectation value tends to zero as well, which implies that the left boundary is described independently from the right boundary.

First, we have to show that the λ_n are bounded between 0 and 1. This is true, because all $|b_n| \in [0, 1]$ (eq. (4.3)) and with eq. (4.6) one can see that $\lambda_n = |b_{n+1}|$.

Then we show that the λ_n are strictly monotone decreasing, i.e.

$$\lambda_{n+1} = \frac{|b_{n+1}|^2}{1 - a_{n+1} \cdot c_{n+1}} = \frac{\lambda_n^2}{1 - a_{n+1} \cdot c_{n+1}} < \lambda_n$$

which is the same as showing

$$1 - a_{n+1} \cdot c_{n+1} > \lambda_n$$

To prove that, we have to consider four cases: $-1 \le a_{n+1} \cdot c_{n+1} < 0$ and $0 < a_{n+1} \cdot c_{n+1} < 1$, $a_{n+1} \cdot c_{n+1} = 1$ and $a_{n+1} \cdot c_{n+1} = 0$.

 $-1 \le a_{n+1} \cdot c_{n+1} < 0$:

In the first case, the condition is fulfilled trivially, as $1 - a_{n+1} \cdot c_{n+1} > 1$ but all λ_n have to be smaller or equal to one, so it is always $1 - a_{n+1} \cdot c_{n+1} > \lambda_n$.

$1 > a_{n+1} \cdot c_{n+1} > 0$:

For this case, let us first show that $a_{n+1} \cdot c_{n+1} \leq \frac{1}{2} \cdot |a_{n+1} + c_{n+1}|$:

$$0 \le (a_{n+1} - c_{n+1})^2 = (a_{n+1} + c_{n+1})^2 - 4 \cdot a_{n+1} \cdot c_{n+1}$$

$$\Leftrightarrow \qquad a_{n+1} \cdot c_{n+1} \le \frac{1}{4} \cdot (a_{n+1} + c_{n+1})^2$$

$$\Leftrightarrow \qquad \sqrt{a_{n+1} \cdot c_{n+1}} \le \frac{1}{2} \cdot |a_{n+1} + c_{n+1}|$$

With the conditions $-1 \le a_{n+1} \le 1$ and $-1 \le c_{n+1} \le 1$, it follows that

$$a_{n+1} \cdot c_{n+1} < \sqrt{a_{n+1} \cdot c_{n+1}} \le \frac{1}{2} \cdot |a_{n+1} + c_{n+1}|.$$

Hence, one can show that

$$1 - a_{n+1} \cdot c_{n+1} > 1 - \sqrt{a_{n+1} \cdot c_{n+1}} \ge 1 - \frac{1}{2} \cdot |a_{n+1} + c_{n+1}| \stackrel{(4.2)}{\ge} |b_{n+1}| = \lambda_n \qquad \Box$$

 $a_{n+1} \cdot c_{n+1} = 1$:

Here, the condition $a_{n+1} \cdot c_{n+1} = 1$ implies that $|a_{n+1} + c_{n+1}| = 2$ and with eq. (4.2) that $|b_{n+1}| = 0$. But this means that applying the Jamiołkowski isomorphism will

not change the CM $\hat{\Gamma}$, or differently speaking $\lambda_n = 0 \ \forall n$.

 $a_{n+1} \cdot c_{n+1} = 0:$

We can see with eq. (4.6) that for this case $b_{n+1} = -b_n^2$. The off-diagonal terms will therefore decay for increasing n as long as $|b_0| < 1$.

So we showed that there is only one case, namely $|b_0| = 1$, where the off-diagonal term is not zero from the beginning and will not strictly monotonously decay with growing system size. In all other cases we can now show that λ_n has a limit for increasing n as it is bounded between 0 and 1 and strictly monotonously decreasing (if not zero right from the start). In the following we will call μ the limit of λ_n for $n \to \infty$ which has the property

$$\lim_{n \to \infty} \lambda_n = \lim_{n \to \infty} \lambda_{n+1} = \lim_{n \to \infty} \lambda_{n-1} = \mu.$$

If we multiply eq. (4.8) with the denominator of the right-hand side, we can take the above limit on both sides. Thus, we get an equation that determines μ :

$$\mu \cdot \left(\mu^2 \cdot (1+\mu)^2 - 2 \cdot \mu^2 - \mu^3\right) = \mu^3$$
$$\Leftrightarrow \quad \mu = 0 \quad \lor \quad \mu = 1 \quad \lor \quad \mu = -2$$

which gives two possible limits, namely $\mu = 0$ and $\mu = 1$, as $\mu = -2$ is not in the range of definition. So if the starting $|b_0| < 1$, the off-diagonal terms of the CM will go to zero and only if $|b_0| = 1$ the off-diagonal part will be 1 for any length of the GfPEPS.

4.1.2. Iterative application of the Jamiołkowski isomorphism

Another way of "growing" the GfPEPS is to do it iteratively. In every step, the resulting auxiliary system consists of k + 1 vertical rings and is described by a $\hat{\Gamma}_k$ as shown in fig. 4.2(b). In the previous section, we combined two $\hat{\Gamma}_n$ with Jamiołkowski's isomorphism, but now we want to group in every step a $\hat{\Gamma}_k$ with a $\hat{\Gamma}_0$ leading to an iterative formula for the entries of the CM. If we go to infinite system size, it makes no difference whether we choose the recursive or the iterative approach. So the limits are the same for both approaches. With the recurrence formula it was easier to show that the off-diagonal term decays for growing system size and with the iterative formula it will be possible to give an expression for the limits of the diagonal entries.

When we group a $\hat{\Gamma}_k$ and a $\hat{\Gamma}_0$ and apply Jamiołkowski's isomorphism the

$$\hat{\mathbf{\Gamma}}_{k+1} = \begin{pmatrix} \mathbf{i}a_k & 0\\ 0 & \mathbf{i}c_0 \end{pmatrix} + \frac{1}{1 - a_0 \cdot c_k} \begin{pmatrix} \mathbf{i} \cdot a_0 \cdot |b_k|^2 & -b_k \cdot b_0\\ \bar{b}_k \cdot \bar{b}_0 & \mathbf{i} \cdot c_k \cdot |b_0|^2 \end{pmatrix}$$

which leads to the iteration formulas

$$a_{k+1} = a_k + a_0 \cdot \frac{|b_k|^2}{1 - a_0 \cdot c_k}$$
(4.9)

$$c_{k+1} = c_0 + c_k \cdot \frac{|b_0|^2}{1 - a_0 \cdot c_k}$$
(4.10)

$$b_{k+1} = -\frac{b_k \cdot b_0}{1 - a_0 \cdot c_k}.$$
(4.11)

In order to give a formula for the values of a_{∞} and c_{∞} for a system with infinitely many fermions in horizontal direction, and hence the limit of the diagonal entries of the CM, we start with showing with mathematical induction that $|c_k|$ is strictly monotone increasing for $c_0, |b_0| \neq 0$, i.e. $|c_{k+1}| > |c_k|$.

1. case, $c_k > 0$: we want to show that $c_{k+1} > c_k \ \forall k$ base step:

$$c_1 = c_0 + c_0 \cdot \frac{|b_0|^2}{1 - a_0 \cdot c_0} > c_0$$
, since $1 - a_0 \cdot c_0 > 0$ and $|b_0| \neq 0$

inductive step: suppose $c_{k+1} > c_k$

$$c_{k+2} = c_0 + c_{k+1} \cdot \frac{|b_0|^2}{1 - a_0 \cdot c_{k+1}} > c_0 + c_k \cdot \frac{|b_0|^2}{1 - a_0 \cdot c_k} = c_{k+1}$$

since $\left(\frac{c_{k+1}}{1 - a_0 \cdot c_{k+1}}\right)^{-1} = \frac{1}{c_{k+1}} - a_0 < \frac{1}{c_k} - a_0 = \left(\frac{c_k}{1 - a_0 \cdot c_k}\right)^{-1}$

2. case, $c_k < 0$: the proof for this case goes along the lines of the proof of the first case with the only difference, that we have to show that $c_{k+1} < c_k$.

This means that the condition $|c_{k+1}| > |c_k|$ holds for $c_0, |b_0| \neq 0$. For every value of k the CM has to satisfy the condition $-\hat{\Gamma}_k^2 \leq 1$, as well, which implies $-1 \leq c_k \leq 1$. So the c_k 's are bounded between -1 and 1 and their absolute value is strictly monotone increasing, so while the sign of the c_k 's does not change during the iteration, there exists a limit c_{∞} for infinite system length which has to fulfill

$$c_{\infty} = c_0 + c_{\infty} \cdot \frac{|b_0|^2}{1 - a_0 \cdot c_{\infty}}$$

$$\Rightarrow \quad c_{\infty} = \frac{1}{2a_0} \left[a_0 c_0 + 1 - |b_0|^2 - \sqrt{\left(a_0 c_0 + 1 - |b_0|^2\right)^2 - 4a_0 c_0} \right].$$

In the previous discussion we grouped the $\hat{\Gamma}_k$ and the $\hat{\Gamma}_0$ together such that the $\hat{\Gamma}_k$ was on the left side and the $\hat{\Gamma}_0$ on the right side. But we could have chosen the other ordering with the $\hat{\Gamma}_0$ always on the left and the $\hat{\Gamma}_k$ on the right which will describe the same system for every k. So we can say that the a_∞ has to have the same form as the c_∞ , we just have to interchange a_0 and c_0 which leads to

$$a_{\infty} = \frac{1}{2c_0} \left[a_0 c_0 + 1 - |b_0|^2 - \sqrt{\left(a_0 c_0 + 1 - |b_0|^2\right)^2 - 4a_0 c_0} \right].$$

We also know from section 4.1.1 that $b_{\infty} = 0$ for $|b_0| \neq 1$. Therefore, we can calculate the limits of every entry of $\hat{\Gamma}_k$ with the initial entries from $\hat{\Gamma}_0$.

4.1.3. Exponential decay of the off-diagonal entries

We have seen in the last two sections that the off-diagonal entry of the CM describing the virtual state is going to zero for increasing system size. We will show now, that the absolute value of the off-diagonal term decays exponentially. We will introduce a decay length and give bounds for the exponential decay and thus this length. One can calculate the bounds on the decay length by the initial values of $\hat{\Gamma}_0$ and c_{∞} .

We consider the iteration formulas 4.9-4.11 from the previous chapter. With these, we can show that the off-diagonal entries in the CM, b_k , decay exponentially. We can give a bound on the decay length for every iterative step. It is

$$e^{-\frac{1}{\xi_{\min}}} \le \left|\frac{b_{k+1}}{b_k}\right| \le e^{-\frac{1}{\xi_{\max}}}$$

with decay lengths $\xi_{\min}, \xi_{\max} > 0$ which we want to specify now. It is

$$\left|\frac{b_{k+1}}{b_k}\right| \stackrel{(4.11)}{=} \frac{|b_0|}{1 - a_0 \cdot c_k}$$

and we have to consider two cases, either $a_0 \cdot c_0 < 0$ or $a_0 \cdot c_0 > 0$, for bounding the exponential decay.

1. case, $a_0 \cdot c_0 < 0$: It follows that $a_0 \cdot c_k < 0$ and $a_0 \cdot c_\infty \le a_0 \cdot c_k \le a_0 \cdot c_0$ and thus

$$\frac{|b_0|}{1 - a_0 \cdot c_k} \ge \frac{|b_0|}{1 - a_0 \cdot c_\infty} =: e^{-\frac{1}{\xi_{\min}}} \quad \text{and} \quad \frac{|b_0|}{1 - a_0 \cdot c_k} \le \frac{|b_0|}{1 - a_0 \cdot c_0} =: e^{-\frac{1}{\xi_{\max}}}$$

2. case, $a_0 \cdot c_0 > 0$: Here, it follows that $a_0 \cdot c_k > 0$ and $a_0 \cdot c_0 \le a_0 \cdot c_k \le a_0 \cdot c_\infty$ and thus

$$\frac{|b_0|}{1 - a_0 \cdot c_k} \ge \frac{|b_0|}{1 - a_0 \cdot c_0} =: e^{-\frac{1}{\xi_{\min}}} \quad \text{and} \quad \frac{|b_0|}{1 - a_0 \cdot c_k} \le \frac{|b_0|}{1 - a_0 \cdot c_\infty} =: e^{-\frac{1}{\xi_{\max}}}$$

The off-diagonal term of $\hat{\Gamma}_k$ is therefore at least exponentially decaying and the decay length is bounded between ξ_{\min} and ξ_{\max} . The definition of these limiting decay lengths depends on the sign of $a_0 \cdot c_0$ but they are always determined by the initial values a_0 , c_0 and $|b_0|$ and by c_{∞} .

Since the c_k tends to c_{∞} , the decay of the b_k is well approximated by $e^{-1/\xi_{\min}}$ for $a_0 \cdot c_0 < 0$ and by $e^{-1/\xi_{\max}}$ for $a_0 \cdot c_0 > 0$ after some iterative steps. The number of steps after which this



Figure 4.3.: Two different cases for the exponential decay of the off-diagonal entry of the CM as in eq. (5.2) for $\lambda = 1/2$ and $N_v = 160$. (a) shows the situation for $\phi = \pi/2$ with a fast decaying off-diagonal term and (b) shows for $\phi = \pi/80$ a slowly decaying off-diagonal entry.

approximation is good depends on the difference between c_0 and c_{∞} and on the average value of the decay length.

Now, we will show for an example the possible behavior of the decay length, which can be calculated for each $\phi = 2\pi k/N_v$, $k = -N_v/2, \ldots, N_v/2$. We get the decay length from a linear fit on the natural logarithm of the off-diagonal values b_k per iteration step as shown in fig. 4.3. We want to consider a model, which we will introduce and discuss more thoroughly in the next chapter. The CM describing the map is given by eq. (5.2) and we choose $\lambda = \frac{1}{2}$. The number of sites in vertical direction is chosen to be $N_v = 160$. This state is special, because it has a non-decaying off-diagonal entry for $\phi = 0$. Therefore, we can compare the behavior for a fast decaying off-diagonal term with a slowly decaying off-diagonal term.

In the case of a fast decay, the region for the decay length given by ξ_{\min} and ξ_{\max} is very narrow as shown in fig. 4.3(a). This means that the decay is very well approximated by the upper bound for the decay length.

In contrast to that, the bound on the decay length is not very good for a slowly decaying off-diagonal entry (fig. 4.3(b)). For such a case, the decay cannot be described by a purely exponential one. But after some initial steps, where there is a decrease in the decay length (or increase, depending on the system), the decay is very well approximated by an exponential one. For our example, one can see that for more than 25 iterations, the decay is very well approximated by ξ_{min} .

4.2. Full problem

If we now consider a system whose CM in general does not have zero entries as in the previous chapter, then the CM of the map is fully described by an 8×8 antisymmetric matrix, due to translational invariance. After Fourier transformation and application of the Jamiołkowski

isomorphism in the vertical dimension it will have the general form

$$\hat{m{\Gamma}}_0 = \left(egin{array}{cc} m{A}_0 & m{B}_0 \ -m{B}_0^\dagger & m{C}_0 \end{array}
ight)$$

where A_0 and C_0 are 2 × 2 skew-hermitian matrices and B_0 is a 2 × 2 complex matrix. Again, we can "grow" the auxiliary system with such a ring to the desired horizontal system size. We believe that even for this full problem, the off-diagonal part in the CM, which is itself a 2 × 2 matrix now, will get smaller, when the GfPEPS gets bigger, except for the special case with $A_0 = C_0 = 0$ and $-\hat{\Gamma}_0^2 = 1$. One can see this as a generalization of the simpler example of the previous section, which made us believe that this is true.

Since we cannot prove our claim for the most general case, we consider a more special case where $A_0 = C_0$ and $[A_0, B_0] = 0$ and $B_0^{\dagger} = e^{i\alpha}B_0$. Here, we can again show that the off-diagonal part vanishes for large systems. The first two conditions ensure that all matrices emerging in the Jamiołkowski isomorphism are diagonalized simultaneously. The last condition ensures that the output of the Jamiołkowski isomorphism again satisfies the same conditions. As in section 4.1.1, we want to calculate $\hat{\Gamma}_k$ recursively.

We will see that Jamiołkowski's isomorphism will not change the structure of the CM and therefore, we can conclude that for a certain k we have

$$\hat{\boldsymbol{\Gamma}}_{k} = \begin{pmatrix} \boldsymbol{A}_{k} & \boldsymbol{B}_{k} \\ -e^{i\alpha_{k}}\boldsymbol{B}_{k} & \boldsymbol{A}_{k} \end{pmatrix}, \quad k = 0, \dots, N_{v}.$$

Another recursive step leads to

$$\hat{\boldsymbol{\Gamma}}_{k+1} = \begin{pmatrix} \boldsymbol{A}_{k} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{A}_{k} \end{pmatrix} + \begin{pmatrix} \boldsymbol{B}_{k} & \boldsymbol{0} \\ \boldsymbol{0} & -\mathrm{e}^{\mathrm{i}\alpha_{k}}\boldsymbol{B}_{k} \end{pmatrix} \cdot \begin{pmatrix} \boldsymbol{A}_{k} & -\mathbb{1} \\ \mathbb{1} & \boldsymbol{A}_{k} \end{pmatrix}^{-1} \cdot \begin{pmatrix} \mathrm{e}^{\mathrm{i}\alpha_{k}}\boldsymbol{B}_{k} & \boldsymbol{0} \\ \boldsymbol{0} & -\boldsymbol{B}_{k} \end{pmatrix}$$

$$= \begin{pmatrix} \boldsymbol{A}_{k} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{A}_{k} \end{pmatrix} + \begin{pmatrix} \boldsymbol{B}_{k} & \boldsymbol{0} \\ \boldsymbol{0} & -\mathrm{e}^{\mathrm{i}\alpha_{k}}\boldsymbol{B}_{k} \end{pmatrix} \cdot \begin{pmatrix} \frac{\boldsymbol{A}_{k}}{\boldsymbol{A}_{k}^{2}+\mathbb{1}} & \frac{\mathbb{1}}{\boldsymbol{A}_{k}^{2}+\mathbb{1}} \\ \frac{-\mathbb{1}}{\boldsymbol{A}_{k}^{2}+\mathbb{1}} & \frac{\boldsymbol{A}_{k}}{\boldsymbol{A}_{k}^{2}+\mathbb{1}} \end{pmatrix} \cdot \begin{pmatrix} \mathrm{e}^{\mathrm{i}\alpha_{k}}\boldsymbol{B}_{k} & \boldsymbol{0} \\ \boldsymbol{0} & -\boldsymbol{B}_{k} \end{pmatrix}$$

$$= \begin{pmatrix} \boldsymbol{A}_{k} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{A}_{k} \end{pmatrix} + \begin{pmatrix} \mathrm{e}^{\mathrm{i}\alpha_{k}}\boldsymbol{B}_{k} \cdot \frac{\boldsymbol{A}_{k}}{\boldsymbol{A}_{k}^{2}+\mathbb{1}} \cdot \boldsymbol{B}_{k} & -\boldsymbol{B}_{k} \cdot \frac{\mathbb{1}}{\boldsymbol{A}_{k}^{2}+\mathbb{1}} \cdot \boldsymbol{B}_{k} \\ \mathrm{e}^{2\mathrm{i}\alpha_{k}}\boldsymbol{B}_{k} \cdot \frac{\mathbb{1}}{\boldsymbol{A}_{k}^{2}+\mathbb{1}} \cdot \boldsymbol{B}_{k} & \mathrm{e}^{\mathrm{i}\alpha_{k}}\boldsymbol{B}_{k} \cdot \frac{\boldsymbol{A}_{k}}{\boldsymbol{A}_{k}^{2}+\mathbb{1}} \cdot \boldsymbol{B}_{k} \end{pmatrix} . \quad (4.12)$$

We have used the fact that

$$\left[\left(\begin{array}{cc} \boldsymbol{A}_k & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{A}_k \end{array} \right), \left(\begin{array}{cc} \boldsymbol{0} & \mathbb{1} \\ -\mathbb{1} & \boldsymbol{0} \end{array} \right) \right] = \boldsymbol{0}$$

which means that the matrices can be diagonalized simultaneously and the inverse can be calculated as above. We can see from eq. (4.12) that $\hat{\Gamma}_{k+1}$ has the same structure as $\hat{\Gamma}_k$ and therefore, we can apply Jamiołkowski's isomorphism recursively. We get the recurrence formulas

$$\boldsymbol{A}_{k+1} = \boldsymbol{A}_{k} + e^{i\alpha_{k}} \boldsymbol{B}_{k} \cdot \frac{\boldsymbol{A}_{k}}{\boldsymbol{A}_{k}^{2} + 1} \cdot \boldsymbol{B}_{k}$$

$$(4.13)$$

$$\boldsymbol{B}_{k+1} = - \boldsymbol{B}_k \cdot \frac{\mathbb{1}}{\boldsymbol{A}_k^2 + \mathbb{1}} \cdot \boldsymbol{B}_k.$$
(4.14)

Since A_{k+1} and B_{k+1} are composed of A_k and B_k and since $[A_k, B_k] = 0$ it is clear that $[A_{k+1}, B_{k+1}] = 0$ is true, as well. Hence, one can show this for every k by mathematical induction. This means that we can diagonalize the matrices in eq. (4.14) simultaneously by a unitary transformation U:

$$\boldsymbol{U}^{-1}\boldsymbol{A}_{k}\boldsymbol{U} = \left(egin{array}{cc} \mathrm{i}\cdot a_{k,1} & 0 \\ 0 & \mathrm{i}\cdot a_{k,2} \end{array}
ight) \quad ext{and} \quad \boldsymbol{U}^{-1}\boldsymbol{B}_{k}\boldsymbol{U} = \left(egin{array}{cc} b_{k,1} & 0 \\ 0 & b_{k,2} \end{array}
ight)$$

with $a_{k,j} \in \mathbb{R}$ and $b_{k,j} \in \mathbb{C}$. This means that the transformed B_{k+1} is diagonal, too and we get a formula for the entries:

$$b_{k+1,j} = -\frac{b_{k,j}^2}{1 - a_{k,j}^2}, \quad j = 1, 2.$$

This formula is the same as in eq. (4.6) for the special case $c_k = a_k$. The $a_{k,j}$ and $b_{k,j}$ fulfill the same properties as the variables in section 4.1.1 due to the property $i\hat{\Gamma}_k \leq \mathbb{1}$. Therefore, the $b_{k,j}$ tend to zero for increasing k by the same arguments as in section 4.1.1. This implies that the whole matrix \boldsymbol{B}_k tends to 0 for increasing k, what we wanted to show here. The only starting values for which the off-diagonal matrix would not tend to zero is for a $|b_{0,j}| = 1$. But then, we have $a_{0,j} = 0$ and will end in the case $\boldsymbol{A} = \boldsymbol{C} = 0$ and $i\boldsymbol{\Gamma} = \mathbb{1}$, for which we expected non-decaying off-diagonal matrices.

5. Numerical calculations

In the previous chapter, we showed that the virtual modes on the left and right boundary decouple for certain auxiliary systems. As stated before, we believe that this is also true for more general systems. We did some numerical calculations for random GfPEPS to test this conjecture and to better understand the properties of the auxiliary system. For these calculations, we considered translational invariant auxiliary systems with $N_v = 160$ sites in vertical direction and $N_h = 100$ sites in horizontal direction. We started with creating a random \mathcal{G} describing the auxiliary map and with this \mathcal{G} we numerically calculated the resulting auxiliary state where we let the system "grow" iteratively, as described in the previous chapters. Then, we assigned a Hamiltonian to this auxiliary state and relate it to the entanglement spectrum of the reduced GfPEPS, as shown in chapter 3.2.

In this chapter, we will present the numerical results for three exemplary auxiliary states. The first and the second example describe maps that do not couple even and odd Majorana operators, i. e. we are in a situation as in chapter 4.1. In the first example, we encounter the most likely case of decaying off-diagonal terms in the Fourier transformed CM for all Fourier angles ϕ . The decay for all ϕ implies that the virtual particles on the left and right boundary also decouple in real space, which means that we can describe the left and right boundary separately for large system lengths. We find that the Hamiltonian for the virtual boundary modes only consists of short-range interactions and therefore we call it quasi-local. The second example is taken from [4]. Here, we have the special case that the off-diagonal terms will not decay for $\phi = 0$. For all other angles ϕ , we still have decaying off-diagonal terms. This non-decaying off-diagonal entry will now result in a coupling of the left and right virtual modes. The third example describe a full map, i. e. we do not have zero entries in \mathcal{G} right from the start and therefore describe a system as in chapter 4.2. For this example, we again find that we have decaying off-diagonal blocks in the Fourier transformed CM for all ϕ . Hence, the left and right boundary can be described separately and we find a quasi-local Hamiltonian.

5.1. Models with non-interacting Majorana operators c_{2i-1} and c_{2j}

In this section, we want to consider GfPEPS whose auxiliary map will be described by a CM that have zero entries for the combination of an even and an odd Majorana operator. As described in chapter 4.1, the calculation of the resulting virtual state separates in two independent problems, one for only even Majorana operators and one for only odd Majorana operators. Therefore, we can consider a $\mathcal{G} \in CM(\mathbb{R}, 4)$ which describes the translational invariant map for the auxiliary system. For our numerical calculations, we choose a random $\mathcal{G} \in CM(\mathbb{R}, 4)$ and calculate the resulting auxiliary state for it, as described before. The resulting auxiliary system is then described by N_v Majorana operators for the left boundary and another N_v Majorana operators for the right boundary.

We encountered for all randomly chosen \mathcal{G} s that we considered a decoupling of the virtual particles at the two boundaries for all angles of ϕ . We will present one of these randomly chosen \mathcal{G} s as an example and discuss the behavior of the auxiliary system and connect its spectrum to the entanglement spectrum.

We also want to discuss the case where we have non-decaying off-diagonal terms in the Γ_k for certain angles of ϕ . Therefore, we will discuss another example which was originally introduced in [4] which shows such a behavior.

5.1.1. Example for decaying off-diagonal entries for all ϕ

As mentioned before, we now present an example which has decaying off-diagonal terms for all Fourier angles ϕ . The translational invariant map for our chosen auxiliary system is described by

$$\boldsymbol{\mathcal{G}} = \begin{pmatrix} 0 & -0.31 & -0.60 & -0.04 \\ 0.31 & 0 & 0.08 & -0.85 \\ 0.60 & -0.08 & 0 & -0.12 \\ 0.04 & 0.85 & 0.12 & 0 \end{pmatrix}.$$
(5.1)

We go to Fourier space and calculate the complete system of N_h horizontal sites. To calculate the resulting auxiliary state, we apply Jamiołkowski's isomorphism iteratively. We can calculate for each possible value of the Fourier angle ϕ the decay length as already mentioned in sec. 4.1.3. In this section, we could also give bounds on the decay length, which we calculated as well. This is shown in fig. 5.1.



Figure 5.1.: Typical decay length of ϕ for the example of eq. (5.1). The blue dots give the average decay length over N_h iterative steps and the red curves give the bound.



Figure 5.2.: Hamiltonian for the left (a) and right (b) boundary for the example of eq. (5.1). One can see that both Hamiltonians show a similar behavior but have different absolute values.

So we have a system, whose off-diagonal terms are decaying for all ϕ . This means, that the correlation between the left and the right boundary decays exponentially. For our example, the maximal decay length is smaller than 9. This means that we can neglect the off-diagonal terms for our system length of $N_h = 100$, because the exponential decay will give a prefactor of at least $e^{-11} \approx 0$ for the off-diagonal term. Therefore, we only need to consider the diagonal terms and can consider the left and right edge separately. We can apply the inverse Fourier transformation to get the covariance matrix $\mathbf{\Gamma}^{\text{out}} \in CM(\mathbb{R}, 2N_v)$ of the complete virtual system. As the virtual modes at the left and right boundary decouple, we can reorder $\mathbf{\Gamma}^{\text{out}}$ such that it is given by

$$\mathbf{\Gamma}^{\mathrm{out}} = \left(egin{array}{cc} \mathbf{\Gamma}_L & 0 \ 0 & \mathbf{\Gamma}_R \end{array}
ight).$$

 Γ_L only contains the expectation values for Majorana operators at the left boundary and Γ_R describes only the right boundary. Due do the translational invariance of the system, Γ_L and Γ_R are both circulant matrices.

We can calculate the resulting Hamiltonian with the CM Γ^{out} and we get a Hamiltonian for the left boundary and one for the right boundary. Since the Γ_L and Γ_R are circulant matrices, the Hamiltonians for the respective boundary will be circulant, too. This implies that the Hamiltonians are described by an N_v -dimensional vector h(n) and the full Hamiltonian is given by

$$H = \sum_{k=1}^{N_v} \sum_{n=0}^{N_v-1} h(n) \cdot c_k c_{\text{mod}(k+n,N_v)}.$$

The resulting Hamiltonians are shown in fig. 5.2. The graphs are antisymmetric around 0 which is due to the antisymmetry of the CM and thus of the Hamiltonian itself. As one can see in fig. 5.2, the biggest terms are those for nearest-neighbor-interactions. All other Hamiltonian terms for



Figure 5.3.: Decay of the Hamiltonian terms for increasing distance n.

a distance n > 1 are fast decaying compared to the nearest-neighbor term. We encounter an almost exponential decay in the Hamiltonian terms for increasing distance n, as well. This is shown in fig. 5.3. Therefore, we call the Hamiltonian for our example quasi-local. The jagged line at the end is due to the numerical precision and has no physical meaning. The Hamiltonian terms for these values are practically zero.

In chapter 3.2 we showed that the spectrum of the auxiliary system is closely related to the spectrum of the reduced density matrix of the GfPEPS. For our chosen example, we do not have a symmetry in our system, such that $C_R = -C_L$. Therefore we have to use the relation in eq. (3.2) to calculate the $\Gamma'_{\text{out},L}$. With this CM, we can calculate the entanglement spectrum which is



Figure 5.4.: Entanglement spectrum of the reduced GfPEPS (a) and its decay (b).

shown in fig. 5.4(a). One can see that this Hamiltonian looks very similar to the Hamiltonian in fig. 5.2 and that they more or less only differ in an overall factor. We also find a good agreement in the decay lengths for increasing distance n for both spectra. This shows that the spectrum of the virtual particles already tells us a lot about the entanglement spectrum. Hence, it is justified to investigate the auxiliary system and deduce properties of the reduced state of the physical system.

5.1.2. Example for a non-decaying off-diagonal entry for one ϕ

Now, we want to discuss a system which has a non-decaying off-diagonal entry for at least one angle ϕ . We choose an example which was introduced in [4] and which describes a chiral topological insulator. For this example, the off-diagonal term at $\phi = 0$ is not decaying for this case, i. e. |b(0)| = 1. But this means that the left and right virtual modes are not decoupled in real space. We will show that we get a diverging Hamiltonian term for the interaction of virtual modes of the left and the right boundary.

We want to discuss the properties of a translational invariant system, whose virtual map is described by the following CM:

$$\mathcal{G} = \begin{pmatrix} 0 & 1-\lambda & -\frac{\lambda}{\sqrt{2}} & \frac{\lambda}{\sqrt{2}} \\ \lambda - 1 & 0 & -\frac{\lambda}{\sqrt{2}} & -\frac{\lambda}{\sqrt{2}} \\ \frac{\lambda}{\sqrt{2}} & \frac{\lambda}{\sqrt{2}} & 0 & 1-\lambda \\ -\frac{\lambda}{\sqrt{2}} & \frac{\lambda}{\sqrt{2}} & \lambda - 1 & 0 \end{pmatrix}.$$
 (5.2)

For such a system, $\lambda \in [0, 1]$ has to be fulfilled to describe a valid Gaussian map. For $\lambda = 0$ and $\lambda = 1$ this describes an uninteresting map from a physical point of view: This \mathcal{G} already describes a pure map and thus there cannot be a physical system included in the map because this would lead to eigenvalues of $i\mathcal{G}$ which are greater than one, which is not allowed. Therefore, we will not discuss these two cases any further.

We present the behavior for $0 < \lambda < 1$ now and construct the resulting auxiliary system as described before. The Fourier transformed CM of a ring is given by

$$\hat{\boldsymbol{\Gamma}}_{0} = \left(\begin{array}{cc} \mathrm{i}a_{0}\left(\phi\right) & b_{0}\left(\phi\right) \\ -b_{0}\left(\phi\right) & -\mathrm{i}a_{0}\left(\phi\right) \end{array} \right)$$

with

$$a_0(\phi) = \frac{-2\lambda^2 \sin(\phi)}{2\left(\lambda^2 - 2\lambda + 2 - 2\left(1 - \lambda\right)\cos(\phi)\right)}$$
(5.3)

and

$$b_0(\phi) = \lambda - 1 - \frac{2\lambda^3 - 2\lambda^2 + 2\lambda^2 \cos(\phi)}{2(\lambda^2 - 2\lambda + 2 - 2(1 - \lambda)\cos(\phi))}.$$
 (5.4)

As one can see from eqs. (5.3) and (5.4), there will be a non-decaying off-diagonal entry only



Figure 5.5.: The average decay length ξ (blue dots) in dependence of ϕ for $\lambda = 1/2$, $N_v = 160$ and $N_h = 100$. The two red curves give the boundary as in sec. 4.1.3. The decay length diverges, i.e. there is no decay of the off-diagonal term for $\phi = 0$.

for $\phi = 0$, while

$$a_0(0) = 0$$
 and $b_0(0) = -1$.

For all other values of ϕ , we find $|b_0(\phi)| < 1$ and the $b_k(\phi)$ converge to zero for increasing k as shown in section 4.1.1. This can also be seen in the average decay length depending on the angle ϕ shown in fig. 5.5. Since the decay length is diverging at $\phi = 0$, there is a non-decaying off-diagonal term. The limits for the decay length can be calculated as in chapter 4.1.3 and they are shown by the red curves in the figure.

The non-decaying term for $\phi = 0$ has a direct consequence for the Hamiltonian. The virtual particles on the left and right boundary are not completely decoupled. We use the inverse Fourier transformation to get a CM in real space again. This CM will have a constant term for the entries corresponding to the product of one auxiliary Majorana operator from the left boundary and one from the right boundary. Hence, the corresponding Hamiltonian will have terms that describe the left boundary and the right boundary, respectively, as before. But now, there will also be one term that describes the interaction between the left and right part. For $\phi = 0$, we can see that

$$\hat{\mathbf{\Gamma}}_k = \left(\begin{array}{cc} 0 & -1\\ 1 & 0 \end{array}\right), \quad \forall k$$

which has eigenvalues i and -i. Since the eigenvalues do not change under Fourier transformation, the CM in real space will have the same spectrum. With $\lambda_j = \tanh\left(\frac{\beta_j}{2}\right)$ (eq. (2.8)), this is connected to a diverging β_j . Therefore, the GfPEPS for this example describes a critical state.

Apart from this diverging term in the Hamiltonian, we have Hamiltonian terms describing only modes on the left boundary and terms describing only right boundary modes. Due to



Figure 5.6.: Hamiltonian for the virtual particles on the left boundary. The Hamiltonian for the virtual particles on the right boundary is the same up to an overall minus sign.

translational invariance, these are again given by

$$\boldsymbol{H} = \sum_{k=1}^{N_v} \sum_{n=0}^{N_v-1} h(n) \cdot c_k c_{\text{mod}(k+n,N_v)}$$

We find for the chosen example that the Hamiltonian for the left part is the same as the Hamiltonian for the right part, up to an overall minus sign. This is due to the symmetry of the $\hat{\Gamma}_0$. When we would choose another ordering of the Majorana operators, such that we interchange the operators for left and right, we would get $-\hat{\Gamma}_0$. In fig. 5.6 we show the left Hamiltonian. Due to the mentioned symmetry in $\hat{\Gamma}_0$, we find that $C_R = -C_L$ and the entanglement spectrum is the same as the auxiliary spectrum in fig. 5.6 up to a factor of 2.

Until now, we considered an auxiliary system with a left and a right boundary. But in the GfPEPS construction from section 2.2.2 we put a boundary ring on each end of the cylinder that has no auxiliary modes in the output port. In the previous section, this was not a concern as the two boundaries were not interacting anyway and putting a boundary ring on one side would not change the spectrum on the other. But as we have interacting boundaries now, we have to take into account the effect of the boundary ring.

In Fourier space, one can understand what happens for the angle $\phi = 0$ where we have nondecaying off-diagonal terms. For this angle, the map is described by a maximally entangled pure state between the two auxiliary modes at each boundary and these are connected with another maximally entangled state to each neighboring site. Therefore, we have a string of maximally entangled modes and putting a boundary state on one side of this system will "teleport" it through the system to the other side. This means that the resulting Hamiltonian of the auxiliary system depends on the edges of the complete system, which can be far apart from the boundary between the two regions.

5.2. Full problem

We will consider now an example for a system whose auxiliary map is described by a general 8×8 CM per site. There are no non-decaying or slowly-decaying off-diagonal terms for all angles of ϕ . So for this example, the left and the right boundary of the auxiliary system will completely decouple again. This means that we will get a Hamiltonian for the left boundary and an independent Hamiltonian for the right boundary. Since we do not have zero values for the combination of even an odd Majorana operators in this CM, the resulting Hamiltonians will contain three terms: one term which only consists of even Majorana operators, one term of only odd Majorana operators and another term an even and an odd operator. We want to show the properties of our chosen example now.

We choose the maximally entangled states between each site as described in chapter 2.2.2. The numerical values for the \mathcal{G} for our chosen example are given in appendix B.

We want that the complete CM $\mathcal{G}_{\text{phys}}$ describing the map from the auxiliary modes to the physical mode is pure, i.e. $-\mathcal{G}_{\text{phys}}^2 = \mathbb{1}$. Therefore, we create a random 10×10 antisymmetric matrix. Then we go to its eigenbasis and set all its eigenvalues to pairs of $\pm i$ and transform it back. With this we get a pure $\mathcal{G}_{\text{phys}}$. We get the \mathcal{G} of our example by taking only the last eight rows and columns of $\mathcal{G}_{\text{phys}}$ corresponding to the auxiliary system.

We get the resulting CM describing the whole system as described before. We will go to Fourier space and combine the vertical auxiliary GfPEPS rings iteratively again. Therefore, we get for every iterative step a

$$\hat{oldsymbol{\Gamma}}_k = \left(egin{array}{cc} oldsymbol{A}_k & oldsymbol{B}_k \ -oldsymbol{B}_k^\dagger & oldsymbol{C}_k \end{array}
ight)$$

with $A_k \in CM(\mathbb{C}, 2)$, $C_k \in CM(\mathbb{C}, 2)$ and a 2 × 2 complex B_k . We can define a decay length, but this time the off-diagonal term is not a number but a matrix. Therefore, for a certain angle ϕ , we take the natural logarithm of the matrix norm of B_k and calculate the decay length with a linear fit on the iterative steps. We suppose that the matrix norm will decay exponentially, although we cannot prove this as for the simple case. The decay length for our example depending on ϕ is shown in fig. 5.7. The matrix norm is equal to the largest singular value of the matrix. If we calculate the decay lengths for both singular values of B_k , we see that the singular value that is the largest for an angle ϕ can be the smallest for another angle ϕ' . This means that both singular values can determine the decay length for different values of ϕ as shown in fig. 5.7 as well.

The fact that we can find a finite decay length for all angles of ϕ shows that the off-diagonal block B_k tends to zero for increasing k. For the chosen example, we see from the decay length that we can neglect the off-diagonal block for our chosen system length of $N_h = 100$ sites.

After the 100 iterative steps, we can take the inverse Fourier transformation to get the resulting



Figure 5.7.: Decay length for the example in eq. (B.1). The blue dots show the decay length calculated with the matrix norm of the off-diagonal block of the CM. The red lines are the decay lengths calculated from the singular values of that off-diagonal block.

CM describing the whole auxiliary system in real space. This is given by

$$\boldsymbol{\Gamma}^{\text{out}} = \left(\begin{array}{cc} \boldsymbol{\Gamma}_L & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\Gamma}_R \end{array}\right)$$

with $\Gamma_L \in CM(\mathbb{R}, 2N_v)$ and $\Gamma_R \in CM(\mathbb{R}, 2N_v)$. With this Γ^{out} we can calculate the corresponding Hamiltonians describing the left and right auxiliary boundary. The Hamiltonians \mathcal{H} will be described by $2N_v \times 2N_v$ diagonal antisymmetric matrices H. We can reorder the vectors of the Majorana operators and the Hamiltonian matrices to get

$$oldsymbol{\mathcal{H}} = \left(egin{array}{cc} oldsymbol{\mathcal{H}}_{1,1} & oldsymbol{\mathcal{H}}_{1,2} \ -oldsymbol{\mathcal{H}}_{1,2}^T & oldsymbol{\mathcal{H}}_{2,2} \end{array}
ight)$$

where $\mathcal{H}_{1,1}$ only contains odd and $\mathcal{H}_{2,2}$ only contains even Majorana operators and $\mathcal{H}_{1,2}$ contains sums of one even and one odd Majorana operator. The corresponding Hamiltonians for the left and the right boundary for our example are shown in fig. 5.8(a)-(c) and fig. 5.8(d)-(f), respectively. The Hamiltonians for this example can be called quasi-local again, since one can see that the terms connecting modes which are separated by a distance n are all tending to zero already for small n.

As one can see in fig. 5.8, we do not have a symmetry for our system leading to $C_R = -C_L$ because otherwise the Hamiltonians for the left and the right boundary should be the same up to a minus sign. Since we do not have such a symmetry, we have to calculate the spectrum of the reduced GfPEPS with eq. (3.2). For that, we naturally assign the CM describing the left boundary to the right auxiliary system and the CM describing the right boundary to the left auxiliary system, i.e. $\Gamma_L = C_R$ and $\Gamma_R = C_L$. With this construction, we will find the



Figure 5.8.: Hamiltonian terms for the left auxiliary boundary (a)–(c) and for the right auxiliary boundary (d)–(f).



Figure 5.9.: Entanglement spectrum of the reduced GfPEPS for the chosen example.

entanglement spectrum of a GfPEPS described by a \mathcal{G} as in eq. (B.1) and $N_v = 160$ sites in horizontal direction and a sufficiently large number of sites in horizontal direction (> 100, as the left and right boundaries decouple in the construction of the auxiliary system). The resulting Hamiltonian \mathcal{H}^{red} is shown in fig. 5.9. We see that the entanglement spectrum and the spectrum of the auxiliary boundary modes looks different for the full problem. For the most general case without any symmetries there seems to be no direct agreement between both spectra. Hence one has to investigate the properties of these systems more thoroughly.

6. Conclusion and outlook

In this thesis we investigated the connection of the entanglement spectrum and the spectrum of the virtual particles at the boundary for Gaussian fermionic PEPS. We started our discussions with an overview on the general construction and calculation of GfPEPS. After that, we were able to show that there is a mapping between the virtual modes at the boundary of a region and the reduced physical state of the GfPEPS of that region. This mapping gives a direct connection between the spectrum of the virtual boundary modes and the entanglement spectrum of the reduced GfPEPS. Then, we focused on the auxiliary system which is found in the reduced state. We could show for certain systems that the coupling between the left and right virtual edge modes decays exponentially with increasing number of horizontal sites. We were also able to give analytical expressions for the entries of the Fourier transformed CM for these cases. Finally, we discussed the previously shown concepts and results for some examples.

We have seen that Gaussian fermionic PEPS are very suitable to describe fermionic systems. The numerical calculations for these kind of states can be done very efficiently. This is different in the PEPS formalism, where one has to introduce truncation methods or other advanced approximative methods in order to be able to simulate these systems. Therefore, we think that a further investigation in the field of GfPEPS is very fruitful. On the one hand, it would be interesting if one could show more analytical properties for the GfPEPS formalism. Understanding the possible behaviors more precisely could lead to knew proposals of interesting states. On the other hand, finding more GfPEPS examples which have non-decaying off-diagonal terms for some Fourier angles ϕ could be of great interest as well, since such states could possess interesting physical properties such as topological order.

A. Additional calculations for Fermionic Gaussian States

A.1. Connection of density matrix and Covariance matrix of a Gaussian state

In this section, we show that a fermionic Gaussian state can be fully described by a covariance matrix Γ . Therefore, we show that Γ and the matrix H in the exponent of the density matrix are brought to block-diagonal form by the same orthogonal transformation O.

A general fermionic Gaussian state is described by a density matrix

$$\boldsymbol{\rho} = \frac{1}{Z} \,\mathrm{e}^{-\frac{\mathrm{i}}{4}\boldsymbol{c}^T \boldsymbol{H} \boldsymbol{c}}$$

where $H \in CM(\mathbb{R}, 2n)$ as in chapter 2.1.1. H can be block-diagonalized by an orthogonal matrix O to

$$\widetilde{H} = \bigoplus \left(\begin{array}{cc} 0 & -\beta_j \\ \beta_j & 0 \end{array} \right)$$

(eqs. (2.6)+(2.7)). Therefore, we can write the density matrix as

$$\boldsymbol{\rho} = \frac{1}{Z} e^{-\frac{i}{4} \boldsymbol{c}^T \boldsymbol{O}^T \widetilde{\boldsymbol{H}} \boldsymbol{O} \boldsymbol{c}}$$

where it is appropriate to introduce transformed Majorana operators $\tilde{c} := Oc$. With these transformed Majorana operators it is easy to give an explicit expression for the density matrix:

$$\rho = \frac{1}{Z} e^{-\frac{i}{4}\widetilde{c}^{T}\widetilde{H}\widetilde{c}} \stackrel{(2.7)}{=} \frac{1}{Z} \exp\left(-\frac{i}{4}\sum_{j=1}^{n}\widetilde{c}_{2j}\beta_{j}\widetilde{c}_{2j-1} - \widetilde{c}_{2j-1}\beta_{j}\widetilde{c}_{2j}\right)$$

$$= \frac{1}{Z}\prod_{j=1}^{n} \exp\left(\frac{i}{2}\beta_{j}\widetilde{c}_{2j-1}\widetilde{c}_{2j}\right) = \frac{1}{Z}\prod_{j=1}^{n}\sum_{k=0}^{\infty}\frac{\left(\frac{i}{2}\beta_{j}\widetilde{c}_{2j-1}\widetilde{c}_{2j}\right)^{k}}{k!}$$

$$= \frac{1}{Z}\prod_{j=1}^{n}\sum_{k=0}^{\infty}\left(\frac{1}{2k!}\cdot\left(\frac{\beta_{j}}{2}\right)^{2k}\cdot\mathbb{1} + \frac{i}{(2k+1)!}\cdot\left(\frac{\beta_{j}}{2}\right)^{2k+1}\cdot\widetilde{c}_{2j-1}\widetilde{c}_{2j}\right)$$

$$= \frac{1}{Z}\prod_{j=1}^{n}\left(\cosh\left(\frac{\beta_{j}}{2}\right)\mathbb{1} + i\cdot\sinh\left(\frac{\beta_{j}}{2}\right)\cdot\widetilde{c}_{2j-1}\widetilde{c}_{2j}\right)$$

since the \tilde{c}_j also form a Clifford algebra and therefore $(\tilde{c}_{2j-1}\tilde{c}_{2j})^2 = -\mathbb{1}$. As the state has to be normalized, i.e. Tr $(\boldsymbol{\rho}) = 1$, the normalization constant Z is

$$Z = 2^n \cdot \prod_{j=1}^n \cosh\left(\frac{\beta_j}{2}\right)$$

The trace can be calculated in the transformed Fock basis similar to eq. 2.1, where the fermionic modes are created and annihilated by some transformed \tilde{a}_j^{\dagger} and \tilde{a}_j . We have to express the Majorana operators in terms of the transformed creation and annihilation operators. See section A.2 for the explicit calculation. We get

$$\boldsymbol{\rho} = \frac{1}{2^n} \prod_{j=1}^n \left(\mathbb{1} + \mathbf{i} \cdot \tanh\left(\frac{\beta_j}{2}\right) \cdot \widetilde{c}_{2j-1} \widetilde{c}_{2j} \right).$$
(A.1)

This density matrix is connected to a CM calculated with the same Majorana operators \tilde{c} [6] and we can use the orthogonal transformation O to obtain a CM described by the normal Majorana operators c.

$$\widetilde{\Gamma}_{ab} = \frac{\mathrm{i}}{2} \operatorname{Tr} \left(\boldsymbol{\rho} \left[\widetilde{c}_{a}, \widetilde{c}_{b} \right] \right) = \frac{\mathrm{i}}{2} \sum_{k,l} \operatorname{Tr} \left(\boldsymbol{\rho} \left[O_{ak} c_{k}, O_{bl} c_{l} \right] \right) = \sum_{k,l} O_{ak} \frac{\mathrm{i}}{2} \operatorname{Tr} \left(\boldsymbol{\rho} \left[c_{k}, c_{l} \right] \right) O_{lb}^{T}$$
$$\Rightarrow \quad \widetilde{\Gamma} = \boldsymbol{O} \cdot \boldsymbol{\Gamma} \cdot \boldsymbol{O}^{T}.$$

Thus, the orthogonal matrix O that brings the antisymmetric matrix H to block-diagonal form, block-diagonalizes Γ , as well.

To calculate the relation between the eigenvalues of the CM and the density matrix, we have to explicitly calculate the $\tilde{\Gamma}_{ab} = \frac{i}{2} \text{Tr} \left(\boldsymbol{\rho} \left[\tilde{c}_a, \tilde{c}_b \right] \right)$ using the $\boldsymbol{\rho}$ from eq. A.1. As $\tilde{\boldsymbol{\Gamma}}$ is block-diagonal, we get the relation

$$\lambda_j = \widetilde{\Gamma}_{2j-1,2j} = \operatorname{iTr}\left(\boldsymbol{\rho}\widetilde{c}_{2j-1}\widetilde{c}_{2j}\right) = \operatorname{tanh}\left(\frac{\beta_j}{2}\right).$$

Therefore, the state can equally be described by its density matrix ρ or by its covariance matrix Γ , since there is a direct relation between Γ and the matrix H in the density matrix.

A.2. Explicit Calculation of traces of the density matrix and in the CM

Here, we show how to calculate a trace in the Fock basis. We encounter these traces in the normalization of the density matrix and in the definition of the CM.

We start with a simple example and consider only one fermionic mode and show how to

calculate the trace of the density matrix and the CM. The density matrix is

$$\boldsymbol{\rho} = \frac{1}{2} \left(\mathbb{1} + \mathbf{i} \cdot \boldsymbol{\lambda} \cdot \widetilde{c}_1 \widetilde{c}_2 \right)$$

with $\tilde{c}_1 = \tilde{a}^{\dagger} + \tilde{a}$ and $\tilde{c}_2 = -i \left(\tilde{a}^{\dagger} - \tilde{a} \right)$ and the Fock basis is $|N_1\rangle = \left(\tilde{a}^{\dagger} \right)^{N_1} |0\rangle$. We already used the relation $\lambda_j = \tanh\left(\frac{\beta_j}{2}\right)$. We can calculate the trace of the density matrix

$$\operatorname{Tr}(\boldsymbol{\rho}) = \frac{1}{2} \sum_{N_1=0}^{1} \langle N_1 | \mathbb{1} + i \cdot \lambda \cdot \widetilde{c}_1 \widetilde{c}_2 | N_1 \rangle$$
$$= \frac{1}{2} \sum_{N_1=0}^{1} \left(\langle N_1 | \mathbb{1} | N_1 \rangle + i \cdot \lambda \cdot \langle N_1 | \widetilde{c}_1 \widetilde{c}_2 | N_1 \rangle \right)$$
$$= \frac{1}{2} \left(2 + i \cdot \lambda \left(\underbrace{\langle 0 | \widetilde{a} \widetilde{a}^{\dagger} | 0 \rangle}_{=1} - \underbrace{\langle 1 | \widetilde{a}^{\dagger} \widetilde{a} | 1 \rangle}_{=1} \right) \right) = 1$$
(A.2)

and similarly the CM

$$\widetilde{\Gamma}_{12} = \mathrm{i}\mathrm{Tr}\left(\boldsymbol{\rho}\widetilde{c}_{1}\widetilde{c}_{2}\right) = \frac{\mathrm{i}}{2}\sum_{N_{1}=0}^{1} \langle N_{1}|(\mathbb{1} + \mathrm{i}\cdot\lambda\cdot\widetilde{c}_{1}\widetilde{c}_{2})\cdot\widetilde{c}_{1}\widetilde{c}_{2}|N_{1}\rangle = \lambda$$
(A.3)

as it should be due to the definition of Γ .

The generalization to more than one fermionic mode is straightforward. It is convenient to use Majorana operators for which the CM is block-diagonal:

$$\begin{split} \widetilde{\mathbf{\Gamma}}_{2j-1,2j} &= \operatorname{iTr}\left(\rho\widetilde{c}_{2j-1}\widetilde{c}_{2j}\right) \\ &= \frac{\mathrm{i}}{2^n}\sum_{N_1\dots N_n=0}^1 \left\langle N_1,\dots,N_n \middle| \prod_{k=1}^n \left(\mathbbm{1} + \mathrm{i}\cdot\lambda_k\cdot\widetilde{c}_{2k-1}\widetilde{c}_{2k}\right)\cdot\widetilde{c}_{2j-1}\widetilde{c}_{2j} \middle| N_1,\dots,N_n \right\rangle \\ &= \frac{\mathrm{i}}{2^n} \left(\prod_{k=1,k\neq j}^n \sum_{N_k=0}^1 \langle N_k | \mathbbm{1} + \mathrm{i}\cdot\lambda_k\cdot\widetilde{c}_{2k-1}\widetilde{c}_{2k} | N_k \rangle \right) \cdot \\ &\cdot \langle N_j | (\mathbbm{1} + \mathrm{i}\cdot\lambda_j\cdot\widetilde{c}_{2j-1}\widetilde{c}_{2j})\cdot\widetilde{c}_{2j-1}\widetilde{c}_{2j} | N_j \rangle \\ \overset{(\mathrm{A}.2),(\mathrm{A}.3)}{=} \frac{\mathrm{i}}{2^n} \cdot 2^{n-1} \cdot 2\lambda_j = \lambda_j \end{split}$$

B. Exemplary CM for the full problem

The CM that describes the auxiliary map for the chosen example in chapter (5.2) is given explicitly by

$$\boldsymbol{\mathcal{G}} = \begin{pmatrix} 0 & g_1 & g_2 & g_3 & g_4 & g_5 & g_6 & g_7 \\ -g_1 & 0 & g_8 & g_9 & g_{10} & g_{11} & g_{12} & g_{13} \\ -g_2 & -g_8 & 0 & g_{14} & g_{15} & g_{16} & g_{17} & g_{18} \\ -g_3 & -g_9 & -g_{14} & 0 & g_{19} & g_{20} & g_{21} & g_{22} \\ -g_4 & -g_{10} & -g_{15} & -g_{19} & 0 & g_{23} & g_{24} & g_{25} \\ -g_5 & -g_{11} & -g_{16} & -g_{20} & -g_{23} & 0 & g_{26} & g_{27} \\ -g_6 & -g_{12} & -g_{17} & -g_{21} & -g_{24} & -g_{26} & 0 & g_{28} \\ -g_7 & -g_{13} & -g_{18} & -g_{22} & -g_{25} & -g_{27} & -g_{28} & 0 \end{pmatrix}$$

(B.1)

with

$g_1 = 0.569333201545209$	$g_2 = 0.208537223574799$
$g_3 = 0.155266101998595$	$g_4 = 0.646028922076655$
$g_5 = 0.328693881825960$	$g_6 = -0.230716591233675$
$g_7 = -0.107246541382728$	$g_8 = 0.011891653082317$
$g_9 = -0.304696132093711$	$g_{10} = -0.011706246083764$
$g_{11} = 0.507940226028796$	$g_{12} = 0.540008300437013$
$g_{13} = 0.045924725091471$	$g_{14} = 0.511044004839846$
$g_{15} = -0.140242406153688$	$g_{16} = -0.044288329520575$
$g_{17} = -0.136032122863447$	$g_{18} = 0.183173258424111$
$g_{19} = -0.300444481126411$	$g_{20} = 0.255502147939725$
$g_{21} = -0.383585058855270$	$g_{22} = 0.491943692109700$
$g_{23} = -0.178339384929541$	$g_{24} = -0.150820918100106$
$g_{25} = -0.167705119793918$	$g_{26} = -0.555669040331032$
$g_{27} = -0.145211855693722$	$g_{28} = 0.286371219961442$

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Acknowledgements

I am deeply grateful to my supervisor, Norbert Schuch, for his guidance through my master thesis. I always admired his great understanding of physics and I gratefully acknowledge the numerous discussions with him.

I also want to say many thanks to Gregor Bransky and Manuel Rispler for their comments on my work and their patience with me.

I want to express my deep gratitude to Barbara Terhal and all other members of the IQI for giving me such a great time during my thesis. It was a pleasure and an honor to work with such friendly and professional people.

Special thanks goes to Eva Kreysing and Susanne Richer, which are great friends and which made every day in the office special.

Last but not least, I am deeply thankful to my friends and family, especially my parents, who always supported me during my studies and who are always there for me. You mean so much to me!