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**Chiral topological PEPS:
understanding Condensed Matter
Physics with Quantum Information
tools.**

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Abstract

Tensor Networks are a tool from quantum information theory to describe many-body quantum systems. It has been shown that states arising from Tensor Networks in 1D (Matrix Product States - MPS) accurately describe ground states of local, gapped Hamiltonians. The same project for higher dimensional systems is currently the subject of great efforts. However, quantum many-body systems in dimension 2 or greater can exhibit much richer behaviour than their one-dimensional counterparts. One of the hallmarks of this is the scarcely understood notion of topological order. It has been shown recently, that Projected Entangled-Pair States (PEPS - Tensor Networks in 2D) can describe chiral topological states, that lie in the ground state manifold of a certain class of gapless Hamiltonians. In this work, we try to perturb the Hamiltonian into a gapped chiral phase. We will then study, whether this gapped, chiral phase can be described in terms of PEPS or how the PEPS-construction has to be modified to accommodate for this kind of behaviour.

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Chapter 1

Introduction

During the last years, the field of Tensor Networks has seen an explosion of results in several directions. This is specially true in the study of quantum many-body systems, both theoretically and numerically. There are many reasons to approach problems in Condensed Matter Physics with this new method.

The general problem in many-body physics is the spectral resolution of Hamiltonians. In this work we will consider systems on a lattice where on each site either spins reside or electrons that are allowed to hop. Although this is already a strong simplification, such systems are believed to accurately describe certain materials and, most importantly, also host some important phenomena observed in continuous Condensed Matter systems such as superconductivity, Bose-Einstein condensation and the Quantum Hall Effect. However, this simplification maintains a big obstacle for the spectral resolution of Hamiltonian: the exponential growth of the Hilbert space associated to the system with the number of particles. Thankfully, not all quantum states in the Hilbert space of a many-body system are equal: some are more relevant than others. The main reason is that many interactions in Nature, and therefore the physical Hamiltonians, are local. This translates into Hilbert spaces in the sense that ground states or lower energy states have some strict properties that characterize them. For example, as we shall see, ground states of gapped and local Hamiltonians obey the so-called area law for the entanglement entropy. This means that the "amount" of entanglement of a state between a compact region and the remainder space scales, for a large enough region, with the boundary, not with the bulk. Intuitively this indicates that the quantum correlations are concentrated on the border of the region, not inside.

Tensor Networks methods represent an appropriate language to describe ground states and lower energy states, states that usually occupy a small but physically relevant corner in the Hilbert space. This description involves networks of interconnected tensors, which in turn capture the relevant entanglement properties of the system on a lattice. Entanglement is already known as a fundamental property in Quantum Information that is a potential resource also for applications such as quantum cryptography or quantum computers. Besides that, it plays an important role also in Condensed Matter: the structure of the entanglement (quantum correlations) between constituents of a system should hold some physical meaning.

In particular, it is expected that this structure depends on various factors, such as the dimensionality of the system, the presence of criticality or correlation lengths. However, the usual approach of describing quantum states by merely give coefficients of wavefunction does not give any intuition about the structure of entanglement. It is desirable, thus, to find a way of representing quantum sates where this information is explicit and easily accessible. As we shall see, Tensor Networks have this information directly available in its description in terms of a network of quantum correlations. In a way, we can think of Tensor Network states as quantum states given in some entanglement representation.

In the present work, we are going to investigate a specific field in Condensed Matter Physics by Tensor Networks, i.e. topological order. A central goal of Condensed Matter is to characterize phases of matters. Some of them, such as magnets and superconductors, can be understood in terms of the symmetries that they spontaneously break, following the very general principles of the Landau-Ginzburg theory. However, in recent decades, it has become apparent that there can exist a more subtle kind of order in the pattern of entanglement of quantum ground states at zero temperature. The concept of topological order was initially introduced to describe the quantum Hall effect. The state of this system, for example, has the fundamental property that it is insensitive to smooth changes in materials parameters and cannot change unless the system passes through a quantum phase transition. These properties can be understood as consequences of the topological structure of the quantum state. One theorized application would be to use topological ordered states as media for quantum computing in a technique known as topological quantum computing. These states, being resistant to local perturbation, can maintain easily the pattern of quantum entanglements, reducing significantly the effect of decoherence.

The notion of topological equivalence is a reference frame for classifying topological systems. The ground states of two gapped Hamiltonians are said to be topological equivalent if they can be adiabatically connected without closing the energy gap. The topological property we are going to study is the Chern number: this is a property that can be explicitly calculated from the state of a system and results to be always an integer. As we will explain, a system with a boundary and with Chern number non-trivial exhibits a chiral edge electronic mode.

The system we will study is a translational invariant gaussian fermionic state on a two dimensional lattice written directly in terms of a given Tensor Network. This state happens to be at the phase transition between different phases with different Chern numbers. The aim of the work is to understand whether the topological states inside the phases can also be described by a Tensor Network. The method used is perturbative: starting from the Hamiltonian on the phase transition that has the given Tensor Network as a ground state, we made a perturbations in the topological phases and find the new ground states; then we will try to perturb the Tensor Network in order to obtain an other Tensor Networks able to describe the new ground states.

The present work is organizes as follow:

- In chapter 2, after a brief introduction of some background notions, we will introduce the general framework of Tensor Networks for spin systems on a lattice: Tensor Networks in one dimension are called Matrix Product State (MPS), while in two or

higher dimensions are called Projected Entangled Pair States (PEPS). In particular we will see their definitions in a constructive approach where the deep spirit of Tensor Networks resides. We are going also to give motivations of their utility, in particular on the possibility of approximate certain class of ground states by them.

- In chapter 3, we are going to extend Tensor Networks to fermionic systems on a two dimensional lattice; in particular we will focus on gaussian fermionic PEPS (GFPEPS), giving their definition and presenting an useful formalism to treat them efficiently.
- In chapter 4, we are going to introduce some notions of Topology in Condensed Matter; in particular, we will define the Chern number that will be the topological property that allows chirality in the GFPEPS studied in the next chapter. Besides, we will present a proof showing that actually a certain class of GFPEPS cannot be chiral.
- In chapter 5, we will studied an example of chiral GFPEPS; it happens that this state appeared as ground state of local gapless Hamiltonian, indicating that the GFPEPS may be interpreted as a point of phase transition between different topological phases. Perturbing this Hamiltonian quadratically, we try to enter in these gapped topological phases computing their ground states: the aim is now to understand if these perturbed chiral ground states of gapped Hamiltonians can be describe by GFPEPS. The proof in the previous chapter is a strong indication that this is not strictly possible, however it does not rule out other possibilities, such as *approximating* them by GFPEPS. Nevertheless, we will find again a negative answer.
- In chapter 6, we will summarize the results of the previous chapter and we will present further possibilities that are left open in order to understand whether the framework of PEPS can be used to describe chiral ground states of gapped Hamiltonians in two dimensions.

Chapter 2

Tensor Networks

2.1 Background

2.1.1 General framework

We will always consider many body quantum systems on D -dimensional lattices with periodic boundary conditions and N sites: eventually, we will take the thermodynamic limit $N \rightarrow \infty$ to study the emergence of critical properties. In particular, in 1-dimension we will consider rings, while in 2-dimension we will study systems on tori. Each lattice site contains a single quantum system: in section 2.2 we will place a d -dimensional spin on each site, i.e. a quantum system living in an Hilbert space \mathbb{C}^d . In the next chapters we will consider instead fermionic systems, in which each site can contain a fermion or, more generally, fermionic modes. Then we will encounter creation and annihilation operators for each mode for each sites that follow the usual anticommutation relations. Another possibility would be to consider bosonic system with commutation relations, but we will not treat this case.

2.1.2 Gapped and gapless Hamiltonians

The lowest energy eigenvectors of an Hamiltonian \hat{H} form a subspace \mathcal{G} of the Hilbert space \mathcal{H} of the system space, the *ground space*. If the ground space is one-dimensional, the ground state is unique, otherwise it is called *degenerate*. The *Hamiltonian gap* is the energy gap from the ground space to the first excited state, so

$$\Delta E = \inf_{|\psi\rangle \in \mathcal{H} \setminus \mathcal{G}} \langle \hat{H} \rangle - E_0, \quad (2.1)$$

where E_0 is the ground state energy. The concepts of gapped and gapless Hamiltonians are valid if we consider a family of Hamiltonians in the thermodynamic limit $N \rightarrow +\infty$. If in this limit $\Delta E \rightarrow 0$, \hat{H} is said to be *gapless*, otherwise it is *gapped*.

2.1.3 Area law

A fundamental question that arises when we consider a state on a lattice is how the entropy of a subregion R scales with the size of that region. The entropy we consider now is the Von Neumann entropy defined in A.2: this is an interesting quantity since it indicates the amount of entanglement (quantum correlations) between R and the remainder space. Naively, one can think that the entropy scales extensively with the size, meaning $S(\rho_R) = \mathcal{O}(R)$, as entropies in statistical mechanics. This is indeed the case for a "random" quantum state: one can define such random vectors using the Haar measure of the unitaries acting on the Hilbert space and finds that the expectation value of the entanglement entropy takes the maximum value $\langle S(\rho_R) \rangle \sim \text{Vol}(R) \log d$ (A.2), up to exponential small correction in the size of the total lattice due to *finite size effects*.

However the extensiveness of the entropy does not hold in specific cases with physical relevance: in such cases, instead, the entropy scales with the boundary of the subsystem, following the so called *area law*. A quantum state on a D -dimensional lattice satisfies the *area law for the Von Neumann entanglement entropy* if for every subregion R of linear size L (and then $\text{Vol}(R) \sim L^D$, where L refers to the number of sites) the entanglement entropy of the reduced state on the subregion scales with the boundary of the region:

$$S(\rho_R) = \mathcal{O}(|\partial R|) \quad (2.2)$$

where $\text{Vol}(\partial R) \sim L^{D-1}$. More mathematically precise, the Area Law makes sense only with a state in the thermodynamic limit, where the number of lattice sites $N \rightarrow +\infty$. Without pretending a formal definition of this limit, a state ψ on the "infinite" lattice is well defined only as a limit of states on a finite lattice, let's say $\{\psi_N\}_{N=1}^{+\infty}$. Let's consider translational invariant states and an arbitrary region R placed anywhere on the lattice. Then, a more precise definition of a state satisfying the area law is given by

$$\exists c \mid \forall N \text{ and } \forall R, S(\rho_{N,R}) \leq c|\partial R|, \quad (2.3)$$

where ∂R is the boundary of R and $\rho_{N,R}$ is the reduce density matrix on R of the quantum state ψ_N :

$$\rho_{N,R} = \text{tr}_{\mathcal{H}_N \setminus \mathcal{H}_R}(|\psi_N\rangle\langle\psi_N|). \quad (2.4)$$

Such an area law has been proven to be valid for a number of cases [5]:

- for any gapped one-dimensional system with a unique ground state;
- for gapped free bosonic and fermionic models (for models where the Hamiltonian can be written as a quadratic polynomial in the creation and annihilation operators) in any dimension;
- for free bosonic models, even for critical (gapless) models for cubic lattice in dimension $D > 1$;
- for tensor networks in any dimension with fixed D , as we will prove in sections 2.2.3 and 2.3.2 in one and two dimension (but the result is easily generalizable to higher dimensions): this is at the very insight why gapped quantum many-body systems can actually be numerically simulated by tensor networks;

- for states defined on a line where the correlations decay exponentially.

We notice that from the first, second and fifth case there is a strong evidence that gapped many-body systems generically satisfy an area law. The fact that all these physically relevant states have this strict property allows us to approximate them by Tensor Networks.

On the other hand, for critical systems, the known result about bosons does not rule out the possibility that other critical systems violate the area law. In particular, it was proven that critical free-fermionic systems do not satisfy an area law: for a cubic lattice in D -dimension, one has

$$S(\rho_{R(L)}) = \mathcal{O}(L^{D-1} \log L), \quad (2.5)$$

which is slightly more than an area law would suggest.

2.2 MPS

The acronym MPS stands for *matrix product state*, that is a convenient way to write a many body quantum state on a 1-dimensional lattice. We specify the definition in the periodic case with position independent matrices (translational invariant (TI) MPS). Precisely, we consider N sites aligned on a ring, labelled by $r \in \mathbb{Z}$, where we make the identification between the sites at $r = N + 1$ and $r = 1$. Each site r contains a spin (physical spin) that lives in an Hilbert space $\mathcal{H}_r = \mathbb{C}^d$ with basis $\{|a_r\rangle\}_{a=1}^d$. A general quantum state $|\psi\rangle \in (\mathbb{C}^d)^{\otimes N}$ can be written in terms of this basis as

$$|\psi\rangle = \sum_{a_1, \dots, a_N=1}^d c^{a_1 \dots a_N} |a_1 \dots a_N\rangle \in (\mathbb{C}^d)^{\otimes N}, \quad (2.6)$$

where $c^{a_1 \dots a_N}$ are complex coefficients. We note that the number of complex parameters needed to specify a generic state is d^N (precisely $d^N - 1$ by the normalization, but we will neglect all the normalizations in the following).

The MPS representation of a state $\psi \in (\mathbb{C}^d)^{\otimes N}$ is given by a set of d matrices labelled by a : $\{M^a\}_{a=1, \dots, d}$, where, for each a , M^a is a $D \times D$ complex matrix with indexes $\alpha, \beta = 1, \dots, D$. D is called the *bond dimension*. In terms of these matrices M^a , the MPS state is written as

$$|\psi\rangle = \sum_{a_1, \dots, a_N=1}^d \text{tr}(M^{a_1} \dots M^{a_N}) |a_1 \dots a_N\rangle \in (\mathbb{C}^d)^{\otimes N}. \quad (2.7)$$

The number of complex parameters needed to specify the MPS is dD^2 .

As we just stated, the definition 2.7 was given for TI MPS with periodic boundary conditions. Actually, we can generalize such definition introducing a family of matrices $\{M_r^a\}_{a=1}^d$ for each site r . So, the trace should be written as $\text{tr}(M_1^{a_1} \dots M_N^{a_N})$, where the subscripts indicate the dependence on the corresponding site. Here the parameters needed are dND^2 . A further generalization is given if we allow different sized matrices: for each r we choose $D_r \times D_{r+1}$ dimensional matrices M_r^a ; the bond dimension is then defined as

$D = \max\{D_r\}_{r=1}^N$. Another possible definition is given for systems with open boundaries (a chain instead of a ring): M_1^a and M_N^a are chosen to be row and column vectors respectively and, instead of the trace, the coefficient is simply given by the number $M_1^{a_1} \cdots M_N^{a_N}$.

The first question that arises is whether every state on an N -lattice can be represented by an MPS. The answer is yes as we are going to prove in a while, but first two comments are in order. Clearly, to write a generic state in this form we would need a bond dimension that includes the exponential freedom of a generic state: then, D should grow exponentially with N if we want to recover all the states in the N -lattice as N increases. Secondly we note that when we talk about the entire Hilbert space $(\mathbb{C}^d)^{\otimes N}$, the geometry of the space (in our case the ring) is totally irrelevant. Indeed, the convenience of MPS does not come from their ability to describe all the states, that is a quite useless property since we would require exponentially increasing bond dimensions: we will see, instead, that the convenient property comes from the fact that the physically relevant quantum states are "well described" by MPS, in the sense that the bond dimension grows only polynomially in the number of sites. We anticipate that for "physically relevant states" we mean usually low energy states of local Hamiltonians over lattices: generally speaking, the entanglement content of these states is usually limited to the correlations between neighbouring sites and this is mainly the property that allow an efficient MPS description.

Nevertheless, we prove now that every state in an Hilbert space $(\mathbb{C}^d)^{\otimes N}$ can be written in the MPS representation with open boundary conditions, i.e. there exist the families of matrices $\{\{M_r^a\}_{a=1}^d\}_{r=1}^N$ (the first family $\{M_1^a\}_{a=1}^d$ is actually composed by row vectors, while the last $\{M_N^a\}_{a=1}^d$ has column vectors) such that

$$|\psi\rangle = \sum_{a_1, \dots, a_N=1}^d M_1^{a_1} \cdots M_N^{a_N} |a_1 \cdots a_N\rangle. \quad (2.8)$$

The proof proceeds by iterative singular value decomposition (A.1) on the lattice sites. We start from the generic state

$$|\psi\rangle = \sum_{a_1, \dots, a_N=1}^d c^{a_1 \cdots a_N} |a_1 \cdots a_N\rangle. \quad (2.9)$$

We define a matrix Ψ_1 $d \times d^{N-1}$ from the coefficients $c^{a_1 \cdots a_N}$ grouping together the indexes (a_2, \dots, a_N) :

$$\Psi_1^{a_1, (a_2, \dots, a_N)} := c^{a_1 \cdots a_N}. \quad (2.10)$$

Then we proceed with the singular value decomposition of Ψ_1 in the conventions of A.1:

$$c^{a_1 \cdots a_N} = \Psi_1^{a_1, (a_2, \dots, a_N)} = \sum_{\alpha_1=1}^{r_1} U_{a_1 \alpha_1}^{a_1} D_{\alpha_1 \alpha_1} (V^\dagger)_{\alpha_1, (a_2, \dots, a_N)} =: \sum_{\alpha_1=1}^{r_1} M_{1 \alpha_1}^{a_1} c_{\alpha_1}^{a_2 \cdots a_N}, \quad (2.11)$$

where we have defined $M_{1 \alpha_1}^{a_1} := U_{a_1 \alpha_1}^{a_1} D_{\alpha_1 \alpha_1}$ and $c_{\alpha_1}^{a_2 \cdots a_N} := (V^\dagger)_{\alpha_1, (a_2, \dots, a_N)}$. We consider $\{M_{1 \alpha_1}^{a_1}\}_{\alpha_1=1}^{r_1}$ as a family of row vectors. We found our first family in (2.8)! The next step consists in the definition of the matrix Ψ_2 of dimension $r_1 d \times d^{N-2}$:

$$\Psi_{2(\alpha_1)}^{a_2, (a_3 \cdots a_N)} := c_{\alpha_1}^{a_2 \cdots a_N}. \quad (2.12)$$

Applying again the singular value decomposition on Ψ_2 , we obtain

$$\begin{aligned}
c^{a_1 \cdots a_N} &= \sum_{\alpha_1=1}^{r_1} M_{1 \alpha_1}^{a_1} \Psi_{2(\alpha_1}^{a_2), (a_3 \cdots a_N)} \\
&= \sum_{\alpha_1=1}^{r_1} \sum_{\alpha_2=1}^{r_2} M_{1 \alpha_1}^{a_1} U_{(\alpha_1}^{a_2)}, \alpha_2 D_{\alpha_2 \alpha_2} (V^\dagger)_{\alpha_2, (a_3, \dots, a_N)} \\
&=: \sum_{\alpha_1=1}^{r_1} \sum_{\alpha_2=1}^{r_2} M_{1 \alpha_1}^{a_1} M_{2 \alpha_1 \alpha_2}^{a_2} c_{\alpha_2}^{a_3 \cdots a_N},
\end{aligned} \tag{2.13}$$

with analogous definitions as above. We then have found also the second family of matrices $\{M_2^{a_2}\}_{a_2=1}^d$. Proceeding in this way iteratively, we finally obtain

$$c^{a_1 \cdots a_N} = \sum_{\alpha_1=1}^{r_1} \cdots \sum_{\alpha_N=1}^{r_N} M_{1 \alpha_1}^{a_1} M_{2 \alpha_1 \alpha_2}^{a_2} \cdots M_{N \alpha_N}^{a_N} = M_1^{a_1} M_2^{a_2} \cdots M_N^{a_N} \tag{2.14}$$

giving the MPS representation (2.8) we wanted.

We notice that at each step, r_i is the Schmidt rank of Ψ_i , an $(r_1 \cdots r_{i-1} d) \times d^{N-i}$ matrix. Then, for an arbitrary state the bond dimension, given by the maximum of r_i , is exponential in N as we expected. For an arbitrary translational invariant state on a finite ring it is also possible to construct a translational invariant MPS [12].

In the following, we will always consider translational invariant tensor networks on lattices with periodic boundary conditions. Since in this form each family of matrices $\{M^a\}_{a=1, \dots, d}$ is independent on the lattice position, we can take the thermodynamic limit $N \rightarrow +\infty$ of the system on the ring to study critical properties of the MPS, maintaining fixed the number of parameters. The same will apply also for PEPS.

2.2.1 Construction of MPS

At a first sight the definition 2.7 of MPS might appear quite intricate, but we present now two equivalent ways to construct it. In particular, we will need these two approaches when we will define gaussian fermionic PEPS: it will be useful to understand the correspondences between the two perspectives so we could easily jump from an approach to the other.

Valence bond construction

To construct the MPS, we assign temporarily a pair of virtual spins of dimension D to each site, called respectively left spin and right spin. We fix the basis of the virtual spins $\{|\alpha\rangle_r^l\}_{\alpha=1}^D \in \mathcal{H}_r^l = \mathbb{C}^D$ for the left spin and $\{|\alpha\rangle_r^r\}_{\alpha=1}^D \in \mathcal{H}_r^r = \mathbb{C}^D$ for the right spin. The initial step for the valence bond construction is the maximally entangled virtual state in which, for each consecutive sites, the state is represented by $|\omega\rangle = \sum_{\alpha=1}^D |\alpha\alpha\rangle$, where the first α refers to the right spin of the left site and the second α to the left spin of the right site (to make it clear, we should write $|\omega_r\rangle = \sum_{\alpha=1}^D |\alpha\rangle_r^r \otimes |\alpha\rangle_{r+1}^l$, however in the following

we will skip these indices). The total initial virtual state is then the tensor product on all the consecutive sites:

$$|\Omega\rangle = \sum_{\alpha_1, \dots, \alpha_N=1}^D |\alpha_N \alpha_1 \alpha_1 \alpha_2 \alpha_2 \dots \alpha_{N-1} \alpha_{N-1} \alpha_N\rangle \in (\mathbb{C}^D \otimes \mathbb{C}^D)^{\otimes N} \quad (2.15)$$

(here the first two indices refer to the first site, the third and the fourth to the second site and so on). The next step of the construction consists in the local linear mapping from the two virtual spins to the physical spin of the same site. The map on each site r is represented by

$$\phi_r = \sum_{a=1}^d \sum_{\alpha\beta=1}^D M_{\alpha\beta}^a |a\rangle_r \langle \alpha\beta|_r =: \text{---} \boxed{M} \text{---}^1. \quad (2.16)$$

Here, we have reinserted the site indices to emphasize the fact that the tensor M is independent on r . Applying the map ϕ_r to each site, we obtain the MPS

$$\begin{aligned} |\psi\rangle &= \left(\bigotimes_{r=1}^N \phi_r \right) |\Omega\rangle = \\ &= \sum_{\gamma_1, \dots, \gamma_N=1}^D \bigotimes_{r=1}^N \sum_{a_r=1}^d \sum_{\alpha_r, \beta_r=1}^D M_{\alpha_r \beta_r}^{a_r} |a_r\rangle \langle \alpha_r \beta_r | \gamma_{r-1} \gamma_r \rangle = \\ &= \sum_{\gamma_1, \dots, \gamma_N=1}^D \bigotimes_{r=1}^N \sum_{a_r=1}^d M_{\gamma_{r-1} \gamma_r}^{a_r} |a_r\rangle = \\ &= \sum_{a_1, \dots, a_N=1}^d \sum_{\gamma_1, \dots, \gamma_N=1}^D M_{\gamma_N \gamma_1}^{a_1} \dots M_{\gamma_{N-1} \gamma_N}^{a_N} |a_1 \dots a_N\rangle = \\ &= \sum_{a_1, \dots, a_N=1}^d \text{tr}(M^{a_1} \dots M^{a_N}) |a_1 \dots a_N\rangle \\ &= \text{---} \boxed{M} \text{---} \boxed{M} \text{---} \dots \text{---} \boxed{M} \text{---} \in (\mathbb{C}^d)^{\otimes N}. \end{aligned} \quad (2.17)$$

From this construction approach to MPS we understand better the meaning of the bond dimension D . We note that for $D = 1$ the initial virtual state in 2.15 is completely separable and the same for our final MPS. Increasing the bond dimension corresponds to increase the entanglement content of the state $|\Omega\rangle$ e consequently of $|\psi\rangle$: in this way, we create an hierarchy between the MPSs described by the value of D .

¹We introduce now a graphical language that is usually used to visualize Tensor Networks easily. A tensor (for us simply a multi-index object like M) is represented by a box; each index, associated to a bra or ket (graphically, we do not distinguish bras and kets since an isomorphism connects them), corresponds to a line, vertical for physical indices and horizontal for virtual ones. The contraction between tensors is represented by connecting the two corresponding blocks.

In the following of this chapter, to avoid misunderstandings, we will keep both the graphical and the standard representation of states and operators.

Fiducial state construction

The other equivalent construction starts from a *fiducial state*, either physical and virtual, $|\phi_r\rangle = M_{\alpha_r\beta_r}^{a_r} |a_r; \alpha_r\beta_r\rangle$ placed on each site. As one can notice, the fiducial state is in one to one correspondence with the local map between virtual and physical of the previous construction. The *total fiducial state* $|\Phi\rangle$ is then the tensor product of the local ones:

$$|\Phi\rangle := \bigotimes_{r=1}^N |\phi_r\rangle. \quad (2.18)$$

The second step consists in a projection acting only on the virtual level. The projector on two consecutive sites is given by $|\omega\rangle\langle\omega|$ with $|\omega\rangle = \sum_{\alpha=1}^D |\alpha\alpha\rangle$ where, as before, first α s of the "ketbra" correspond to the right spin of the left site and vice versa for the second α s. The total projector is then

$$|\Omega\rangle\langle\Omega| = \sum_{\alpha_1, \dots, \alpha_N=1}^D |\alpha_N\alpha_1\alpha_1\alpha_2 \cdots \alpha_{N-1}\alpha_{N-1}\alpha_N\rangle \sum_{\beta_1, \dots, \beta_N=1}^D \langle\beta_N\beta_1\beta_1\beta_2 \cdots \beta_{N-1}\beta_{N-1}\beta_N|.$$

Finally, the final physical state is obtained tracing out the virtual spins:

$$|\psi\rangle\langle\psi| = \text{Tr}_V(|\Omega\rangle\langle\Omega| \bigotimes_{r=1}^N |\phi_r\rangle \bigotimes_{s=1}^N \langle\phi_s| |\Omega\rangle\langle\Omega|). \quad (2.19)$$

Clearly, when we sum over the basis vectors of the virtual space, the above expression simplifies:

$$|\psi\rangle\langle\psi| = \langle\Omega| \bigotimes_{r=1}^N |\phi_r\rangle \bigotimes_{s=1}^N \langle\phi_s| |\Omega\rangle \quad (2.20)$$

and then

$$|\psi\rangle = \langle\Omega| \bigotimes_{r=1}^N |\phi_r\rangle, \quad (2.21)$$

that corresponds to the state obtain in the valence bond construction approach. As can be noticed, at the end the two methods are simply related by the exchange of bras with kets in the virtual Hilbert space. When we will introduce fermionic PEPS, we will follow the fiducial state construction that appears more intuitive than the other approach.

2.2.2 Parent Hamiltonians

Given an MPS state $|\psi\rangle$, we can always easily construct a local and frustration free Hamiltonian that has $|\psi\rangle$ as ground state. We write it as

$$H = \sum_r h_r, \quad (2.22)$$

where each term h_r acts on the neighbouring sites of r , up to a range $\ll N$ (in particular independent on N). *Frustration free* Hamiltonian means that every ground state of H is

also ground state of each local term h_r . Equivalently, a particular ground state of H is ground state of each h_r : indeed, in the case of degenerate ground states, it cannot happen that a state is ground state of H and not of a certain h_r while another is ground state of every h_r .

We proceed with the construction of a parent Hamiltonian for a generic MPS, where the local h_r acts on two neighbouring sites. We start constructing the term h_1 acting on sites 1 and 2. The reduce density matrix for these two sites is

$$\rho_2 = \sum_{\substack{a_1, a_2, b_1, b_2, \\ a_3, \dots, a_N}} \text{tr}(M^{a_1} M^{a_2} M^{a_3} \dots M^{a_N}) |a_1, a_2\rangle \langle b_1, b_2| \text{tr}(M^{b_1} M^{b_2} M^{a_3} \dots M^{a_N})^* \quad (2.23)$$

We define a set S_2 of states in $(\mathbb{C}^d)^{\otimes 2}$ in the following way

$$S_2 := \left\{ \sum_{a,b} \text{tr}(M^a M^b X) |a, b\rangle \mid X \in \mathcal{L}(\mathbb{C}^D) \right\} = \left\{ \left[\begin{array}{c} \text{---} \\ | \\ M \\ \text{---} \\ \text{---} \\ | \\ M \\ \text{---} \\ \text{---} \\ X \\ \text{---} \\ | \\ M \\ \text{---} \\ M \\ \text{---} \\ \text{---} \\ | \\ X \end{array} \right] \mid X \right\}. \quad (2.24)$$

We prove now that $\text{Supp}(\rho_2) \subseteq S_2$. The support of a matrix is the orthogonal space to the kernel: so we just have to prove that $S_2^\perp \subseteq \text{Ker}(\rho_2)$. A generic element of $|v\rangle \in (\mathbb{C}^d)^{\otimes 2}$ of S_2^\perp satisfies

$$\sum_{a,b} \text{tr}(M^a M^b X) \langle v | a, b \rangle = \left[\begin{array}{c} v \\ | \\ M \\ \text{---} \\ \text{---} \\ | \\ X \\ \text{---} \\ | \\ M \\ \text{---} \\ M \\ \text{---} \\ \text{---} \\ | \\ X \end{array} \right] = 0, \quad \forall X \in \mathcal{L}(\mathbb{C}^D). \quad (2.25)$$

Then $|v\rangle \in \text{Ker}(\rho_2)$ since, from 2.23 and 2.25,

$$\sum_{a,b} \text{tr}(M^a M^b M^{a_3} \dots M^{a_N}) \langle v | a, b \rangle = 0. \quad (2.26)$$

We define now

$$\tilde{h} := \mathbb{1}^{\otimes 2} - \Pi_{S_2}, \quad (2.27)$$

where Π_{S_2} is the projector on the subspace S_2 and $\mathbb{1}$ is the identity operator on one single site. We notice that $\tilde{h} \geq 0$ since a projector has eigenvalues 0 and 1. From the property $\text{Supp}(\rho_2) \subseteq S_2$ we have that if $|\phi\rangle \in \text{Supp}(\rho_2)$ then $\tilde{h}|\phi\rangle = 0$. In particular, our MPS

$|\psi\rangle \in \text{Supp}(\rho_2)$ ², so $\tilde{h}|\psi\rangle = 0$. If now we construct \tilde{h} for every pair of neighbouring sites, the local term h_r that we wanted to obtain is

$$h_r = \mathbb{1}^{\otimes i-1} \otimes \tilde{h} \otimes \mathbb{1}^{\otimes N-i-1}. \quad (2.28)$$

Each of these local and positive terms annihilate the MPS $|\psi\rangle$, so we end up with a local frustration free hamiltonian that has $|\psi\rangle$ as ground state.

The above parent Hamiltonian has been constructed by local terms $\mathbb{1}^{\otimes 2} - \Pi_{S_2}$. Actually, the only sufficient requirement to have a local and frustration free Hamiltonian is to find an operator that is null on the set S_2 . In particular, from an operator $\hat{A} \in \mathcal{L}((\mathbb{C}^d)^{\otimes 2})$ that annihilates S_2 we can construct a local term of the Hamiltonian by

$$\tilde{h} = \hat{A}^\dagger \hat{A}. \quad (2.29)$$

We notice that \tilde{h} is hermitian and semi-positive³. To find such an operator we propose the following method. Consider the following incomplete MPS on two sites: we place the fiducial state on the first and second site and we project only the right virtual spin on the first site with the left virtual spin on the second site, obtaining the virtual+physical state

$$|\varphi_2\rangle = \text{---} \boxed{\varphi_2} \text{---} := \sum_{a,b} \sum_{\alpha,\beta,\gamma} M_{\alpha\beta}^a M_{\beta\gamma}^b |a, b; \alpha, \gamma\rangle = \text{---} \boxed{M} \text{---} \boxed{M} \text{---}. \quad (2.30)$$

By the Schmidt decomposition, we can bipartite this state between the physical and virtual spins, obtaining

$$|\varphi_2\rangle = \sum_i |P_i\rangle |V_i\rangle = \sum_i \begin{array}{|c|} \hline P_i \\ \hline V_i \\ \hline \end{array}, \quad (2.31)$$

for some orthogonal $|P_i\rangle \in (\mathbb{C}^d)^{\otimes 2}$ and orthonormal $|V_i\rangle \in (\mathbb{C}^D)^{\otimes 2}$; we absorb the Schmidt coefficients in $|P_i\rangle$. Now we take the trace over the virtual spins:

$$\varrho_2 = \sum_i |P_i\rangle \langle P_i| = \sum_i \begin{array}{|c|} \hline P_i \\ \hline P_i \\ \hline \end{array}. \quad (2.32)$$

²This is a quite obvious property: every pure state $|\psi\rangle$ is in the support of every density matrices ρ_A constructed from it or, more precisely, on the support of $\rho_A \otimes \mathbb{1}_B$, where $\mathbb{1}_B$ is the identity on \mathcal{H}_B , the complementary Hilbert space respect to \mathcal{H}_A . In fact, if $|\psi\rangle$ is our state, we can decompose it by the Schmidt decomposition on the generic bipartition AB : $|\psi\rangle = \sum_i \lambda_i |\phi_i\rangle |\phi'_i\rangle$, with the usual conventions reported in A.1. If we trace out the subsystem B , we obtain $\rho_A = \text{tr}_B(|\psi\rangle \langle \psi|) = \sum_i \lambda_i^2 |\phi_i\rangle \langle \phi_i|$. So, if $|v\rangle \in \text{Supp}(\rho_A \otimes \mathbb{1}_B)^\perp = \text{Ker}(\rho_A) \otimes \mathcal{H}_B$, then $\langle v | (|\phi_i\rangle \otimes |\phi'_i\rangle) \rangle = 0 \forall i$ and $\forall |\phi\rangle \in \mathcal{H}_B$. This implies $\langle v | \psi \rangle = 0$ and then $|\psi\rangle \in \text{Supp}(\rho_A \otimes \mathbb{1}_B)$.

³ $\forall |\psi\rangle, \langle \psi | \tilde{h} | \psi \rangle = \langle \psi | \hat{A}^\dagger \hat{A} | \psi \rangle = \|\hat{A}|\psi\rangle\|^2 \geq 0$.

We claim that in order to satisfy $\hat{A}S_2 = 0$, it is sufficient to satisfy

$$\hat{A}\varrho_2 = \sum_i \begin{array}{c} \text{---} \\ | \\ \boxed{A} \\ | \\ \boxed{P_i} \\ | \\ \boxed{P_i} \\ | \\ \text{---} \end{array} = 0. \quad (2.33)$$

Supposing that this operator exists, now we are going to prove that $\hat{A}S_2 = 0$. From the last equality, we conclude that

$$\hat{A}|P_i\rangle = \begin{array}{c} \text{---} \\ | \\ \boxed{A} \\ | \\ \boxed{P_i} \\ | \\ \text{---} \end{array} = 0 \quad (2.34)$$

since $|P_i\rangle$ are orthogonal due from the Schmidt decomposition. A generic element in S_2 is written as $\sum_{a,b} \text{tr}(M^a M^b X)|a, b\rangle$ with $X \in \mathcal{L}(\mathbb{C}^D) \simeq (\mathbb{C}^D)^{\otimes 2}$ (then we can consider the state $|X\rangle$ from the isomorphism). We just need to show then $\hat{A}\sum_{a,b} \text{tr}(M^a M^b X)|a, b\rangle = 0$ or, rewriting in terms of $\langle X|$:

$$\hat{A} \sum_{a,b} \sum_{\alpha,\beta,\gamma} \langle X|M_{\alpha\beta}^a M_{\beta\gamma}^b |a, b; \alpha, \gamma\rangle = \begin{array}{c} \text{---} \\ | \\ \boxed{A} \\ | \\ \boxed{M} \quad \boxed{M} \\ | \\ \boxed{X} \\ | \\ \text{---} \end{array} = 0. \quad (2.35)$$

Using (2.30) and (2.31), we can simply conclude for a generic X :

$$\begin{aligned} \hat{A} \sum_{a,b} \text{tr}(M^a M^b X)|a, b\rangle &= \hat{A}\langle X|\varphi_2\rangle = \begin{array}{c} \text{---} \\ | \\ \boxed{A} \\ | \\ \boxed{\varphi_2} \\ | \\ \boxed{X} \\ | \\ \text{---} \end{array} \\ &= \hat{A}X \left(\sum_i |P_i\rangle|V_i\rangle \right) = \sum_i \begin{array}{c} \text{---} \\ | \\ \boxed{A} \\ | \\ \boxed{P_i} \\ | \\ \boxed{V_i} \\ | \\ \boxed{X} \\ | \\ \text{---} \end{array} \\ &= 0. \end{aligned} \quad (2.36)$$

We conclude that finding operators that satisfy (2.33), we can construct easily local and frustration free parent Hamiltonians. This will be the method we will use for gaussian fermionic PEPS.

We notice that the parent Hamiltonians we constructed in this section could have degenerate ground states. Nevertheless, there exist some results ([14]) that assures some control on the ground state: in particular, if the MPS is *injective*, that means that the map \mathcal{E} (2.16) from the virtual system to the physical one is injective, then the parent Hamiltonian constructed in the way above has an unique ground state, our MPS. With a weaker condition on the initial MPS, i.e. that the MPS is G -injective with G a finite group⁴, the degeneracy of the ground state of the parent hamiltonian is equal to the number of conjugacy classes of G (that is also the number of irreducible representations of G) (see 2.16 for more details). The control on the degeneracy of the ground state is an important property when we go in the thermodynamic limit: it is proved, indeed, that the local parent Hamiltonian we can construct from the injective and G -injective MPS is gapped.

2.2.3 Properties of MPS

- (*Area Law*) MPSs satisfy the Area Law defined in 2.1.3. Notice that we need to consider a translational invariant MPS in order to be able to extend an MPS in the thermodynamic limit. To prove the statement we try to find an upper bound for the entanglement entropy of a subregion of our 1-dimensional lattice. Let's take a generic MPS described by the family of matrices $\{A^i\}_{i=1}^d$ with bond dimension D on an arbitrary N -sites lattice. We consider a subchain of length L and rewrite the MPS $|\psi\rangle$ as a sum of states belonging to the region L and the region $N \setminus L$:

$$|\psi\rangle = \sum_{\alpha, \beta=1}^D |\psi_L(\alpha, \beta)\rangle |\psi_{N \setminus L}(\alpha, \beta)\rangle \quad (2.37)$$

where

$$\begin{aligned} |\psi_L(\alpha, \beta)\rangle &:= \sum_{a_1, \dots, a_L=1}^d (M^{a_1} \dots M^{a_L})_{\alpha\beta} |a_1 \dots a_L\rangle, \\ |\psi_{N \setminus L}(\alpha, \beta)\rangle &:= \sum_{a_{L+1}, \dots, a_N=1}^d (M^{a_{L+1}} \dots M^{a_N})_{\beta\alpha} |a_{L+1} \dots a_N\rangle. \end{aligned} \quad (2.38)$$

The reduced density matrix is then in the simple form

$$\rho_L = \sum_{\alpha, \beta, \alpha', \beta'=1}^D X_{\alpha'\beta'}^{\alpha\beta} |\psi_L(\alpha', \beta')\rangle \langle \psi_L(\alpha', \beta')| \quad (2.39)$$

⁴We introduce the definition of G -injectivity for completeness, but we skip further details. Given a finite group G with unitary representation U_g , we say that an MPS tensor M is G -injective if

- $\forall a, g, U_g M^a U_g^\dagger = M^a$ and
- the map \mathcal{E} has a left inverse on the subspace $\mathcal{S} = \{X | [X, U_g] = 0, \forall g\}$ of invariant matrices, i.e. $\exists \mathcal{E}^{-1} | \mathcal{E}^{-1} \mathcal{E} = \mathbb{1}_{\mathcal{S}}$.

with certain coefficients $X_{\alpha'\beta'}^{\alpha\beta}$. We note that $\text{rk}(\rho_L) \leq D^2$. We know that the Von Neumann entanglement entropy is bounded by $\log \text{rk}(\rho_L)$ (see A.2), then

$$S(\rho_L) \leq \log \text{rk}(\rho_L) \leq 2 \log D. \quad (2.40)$$

We notice that this upper bound is independent on N and on L , then the MPS satisfies the 1-dimensional Area Law $S(\rho_L) = \mathcal{O}(\log D)$.

- (*Correlations*) It can be show [10] that the correlation functions of an MPS decay always exponentially with the separation distance. A correlation function is usually defined as the correlation for between two local observables defined for each r :

$$C(r) := \langle O_s O'_{s+r} \rangle - \langle O_s \rangle \langle O'_{s+r} \rangle, \quad (2.41)$$

where O_r and O'_r are the local observables acting on the r -site or in the neighbourhood of it. $C(r)$ is independent on s if the state and the observables are translational invariant. For every MPS then we have:

$$C(r) \sim e^{-\frac{r}{\xi}} \quad (2.42)$$

where ξ is the correlation length given by

$$\frac{1}{\xi} := \lim_{r \rightarrow +\infty} \frac{1}{r} \log(C(r)). \quad (2.43)$$

The exponential decay is typical in ground states of gapped systems: this is an indication that MPS are able to approximate well this type of states.

- (*Ground states*) It is proved [17] that states that satisfies an area law in one dimension can be well approximated by MPS. In particular, in section 2.1.3 we said that states with exponentially decaying correlations satisfies an area law. In particular then, ground states of local gapped Hamiltonians are well described by MPS, since they have exponentially decaying correlations. Actually, MPS can do some more work: there exists an efficient scalable representation also for ground states of critical (gapless) systems in term of MPS [17]. Operationally, the possibility to approximate ground states of critical systems does not means that we can find the real correlations by an MPS. Usually, what can be done is computing the correlations of a critical state using an MPS representation on N sites up to a certain range: if one wanted to find correlations on longer distances, one should increase sufficiently N and, then, D (but at maximum only polynomially as we shall show below). We remark the fact that this does not mean that MPS can describe critical systems, but only that they can approximate them for each N with a bond dimension that not does not diverge exponentially.

Nevertheless, for both gapped and gapless system, MPS are quite efficient in the following precise way: let's consider a family of states $|\phi_N\rangle$, for increasing N , that we

want to approximate with an MPS $|\psi_N(D_N)\rangle$ with bond dimension $D(N)$ such that the error made by the approximation is bounded by

$$\| |\phi_N\rangle - |\psi_N(D_N)\rangle \| \leq \frac{\epsilon}{N} \tag{2.44}$$

with a fixed ϵ . Then it can be show [17] that the bond dimension scales polynomially if the system satisfies an area-law for a Renyi entanglement entropy S_α (A.3):

$$D(N) \sim \mathcal{O}(N^{f(\alpha)}). \tag{2.45}$$

With some corrections, always polynomial in N , these results hold also for ground states of critical systems that does not satisfy an area law, for example free-fermionic systems for which

$$S(\rho_L) = \mathcal{O}(\log L). \tag{2.46}$$

2.3 PEPS

Projected Entangled Pair States (PEPS) constitute a natural generalization of MPS to two and higher bond dimensions, motivated by the quantum information perspective on MPS which views them as arising from virtual entangled pairs between nearest neighbours. There has not yet been a formal result that PEPS approximate efficiently all ground states of gapped local Hamiltonians, as MPS do in one dimension . Even if less understood than MPS, PEPS allows a much larger variety of different behaviour, in particular they can describe critical systems. For example, just in chapter 5 we will introduce a fermionic PEPS, ground state of a gapless Hamiltonian, with polynomially decaying correlations. Furthermore, to stay in the framework of spin systems, in [18] it was shown that there exists a spin PEPS with power-law decay of two-points correlation functions, something that is not possible with MPS as we have seen.

The definition of PEPS resembles the one for MPS, extended in two dimensions. Now the matrices M^a have four virtual indexes ($M_{\alpha\beta\gamma\delta}^a$, referred, respectively, to the up, down, left, right virtual mode), one for each neighbouring site in the lattice with which they will be contracted. A state $|\psi\rangle$ is a translational invariant PEPS on a N-sites lattice ($L \times L$) of

⁵Here, to measure the distance between the two states, we use the usual norm of vector.

⁶The factor N at the denominator is introduced to avoid that the error made in the measurement of extensive observables increases with N .

bond dimension D if it can be written as ⁷

$$\begin{aligned}
|\psi\rangle = & \sum_{\substack{v_{1,1}, \dots, v_{L,L} = 1 \\ h_{1,1}, \dots, h_{L,L} = 1}}^D \sum_{a_{1,1}, \dots, a_{L,L} = 1}^d \\
& M_{v_{L,1}v_{1,1}h_{1,L}h_{1,1}}^{a_{1,1}} \quad M_{v_{L,2}v_{1,2}h_{1,1}h_{1,2}}^{a_{1,2}} \quad \dots \quad M_{v_{L,L}v_{1,L}h_{1,L-1}h_{1,L}}^{a_{1,L}} \\
& \vdots \\
& M_{v_{L-1,1}v_{1,1}h_{L,L}h_{L,1}}^{a_{L,1}} \quad M_{v_{L-1,2}v_{1,2}h_{L,L}h_{L,2}}^{a_{L,2}} \quad \dots \quad M_{v_{L-1,L}v_{1,L}h_{L,L-1}h_{L,L}}^{a_{L,L}}
\end{aligned} \tag{2.47}$$

$|a_{1,1}a_{1,2} \dots a_{L,L}\rangle$

2.3.1 Construction of PEPS

The formula above is much more complicated than the philosophy beyond the tensor network. For this reason, PEPS are usually defined directly by their construction that resemble their physical meaning. Following the fiducial state construction, there are three steps to perform:

- place the fiducial state

$$\sum_{a=1}^d \sum_{\alpha\beta\gamma\delta=1}^D M_{\alpha\beta\gamma\delta}^a |a\alpha\beta\gamma\delta\rangle = \text{---} \boxed{M \bullet} \text{---} \tag{2.48}$$

on each site;

- projecting over all the bonds (including the bonds between the last and first column and the last and first row to close the boundary); the projectors will be in the form $|\omega\rangle\langle\omega|$ with $|\omega\rangle = \sum_{\alpha=1}^D |\alpha\rangle$: if the bond is vertical (*resp.* horizontal), the first index α refers to the virtual up (*resp.* left) mode of the site below (*resp.* on the right) and the second to the virtual down (*resp.* right) mode of the site above (*resp.* on the left);
- tracing out the virtual space.

⁷For PEPS, we slightly change the conventions for the graphical language of Tensor Networks: the four bonds attached to a box correspond to the virtual indexes, while the physical ones are represented by \bullet , indicating a bond that comes out from the plane. In 2.47 we notice the dotted lines from the first and last row (*resp.* column) that close the boundaries.

By the above construction, one can now understand expression (2.47). Again, as for MPS, the procedure is the same if we simply place the fiducial state on each site and apply all the "bra" projectors ($\langle \omega |$) for each bond. However, the three steps above appears more clear in the framework of fermionic PEPS, as we will see.

We skip now the construction of the parent, local, frustration free Hamiltonian since it would be exactly identical to the procedure made for MPS. The only difference regards the fact that one should take a 2×2 plaquette in two dimension, instead of 2 consecutive sites, to construct a local hamiltonian term that acts on it. As in the case of MPS, G -injectivity can be defined for PEPS leading to some control on the ground state of the parent Hamiltonian constructed above. In the case of PEPS, there is not a formal result that connects the injectivity/ G -injectivity with the gappedness as in the case of MPS. Nevertheless, the control on the degeneracy of the ground state is considered a strong indication for it.

2.3.2 Properties of PEPS

- (*Area Law*) Analogously to MPS, also PEPS satisfies an area law scaling of the entanglement entropy. The proof of this fact follows exactly the case for MPS, except that now we should take a 2-dimensional region, let's say $L \times L$. The sum in (2.37) then runs over D^{4L} terms instead of D^2 since the inside region and the outside one are connected by $4L$ bonds. From the same type of bounds made before, we end up with the following area law:

$$S(\rho_L) = \mathcal{O}(L \log D). \quad (2.49)$$

- (*Ground states*) Unlike MPS, PEPS can handle polynomially-decaying correlations. As already anticipate, this property is important since correlation functions that decay polynomially are characteristic of critical points, where the correlation length is infinite and the system is scale invariant. Unfortunately, on the other hand, we have no general statements that show that ground states of gapped systems can be efficiently written as PEPS, even if all the numerics done so far seem to indicate this, at least in physical cases.

Chapter 3

Gaussian fermionic PEPS

In this chapter we introduce the definition of a gaussian fermion states and some useful techniques to deal with them. In particular, we are interested in restricting our study to gaussian fermionic PEPS (GFPEPS): in this way, all the calculations can be done analytically since we just need to deal with a small number of degrees of freedom in the correlation matrix that describes our state completely.

3.1 FPEPS

We proceed now with the definition of fermionic PEPS in two dimensions: in analogy with PEPS, fPEPS are well suited to describe fermionic system with local interactions.

Before introducing fPEPS, we briefly review what we mean in general for fermionic systems. After that, we will proceed with the construction of fPEPS following the same structure we used for PEPS.

3.1.1 Fermionic systems

We want to describe a system composed of fermions that can individually be in one of N possible states that we called *modes*. For each mode $i = 1, \dots, N$, we describe it by a creation (\hat{a}_i^\dagger) and an annihilation (\hat{a}_i) operator that follow the standard anticommutation rules

$$\begin{aligned}\{\hat{a}_i, \hat{a}_j^\dagger\} &= \delta_{ij}, \\ \{\hat{a}_i, \hat{a}_j\} &= 0, \\ \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} &= 0.\end{aligned}\tag{3.1}$$

A fermionic state is described by a vector in the Fock space $\mathcal{F}(N)$ where these operators act. Defining the vacuum state $|0\rangle$ such that $\hat{a}_i|0\rangle = 0$ for every i , an orthonormal basis for $\mathcal{F}(N)$ is given by:

$$|n_1, \dots, n_N\rangle := (\hat{a}_1^\dagger)^{n_1} \dots (\hat{a}_N^\dagger)^{n_N} |0\rangle,\tag{3.2}$$

We notice that, due to the anticommutation relations, for each i , n_i can only take the values 0 or 1 in order to obtain vectors different from 0: then, we obtain 2^N basis vector that generate the Fock space $\mathcal{F}(N)$. We interpret these n_i 's as the number of fermions (0 or 1) that occupy the i -th mode.

In the following, we will extensively use *Majorana operators* (\hat{c}_j , $j = 1, \dots, 2N$) to describe fermionic systems. There are two Majorana's operators defined for each mode, simply given by

$$\begin{aligned}\hat{c}_{2i} &:= \hat{a}_i^\dagger + \hat{a}_i, \\ \hat{c}_{2i-1} &:= -i(\hat{a}_i^\dagger - \hat{a}_i).\end{aligned}\tag{3.3}$$

From the anticommutation relations between creation and annihilation operators, we find the following relations for the Majorana's operators

$$\{\hat{c}_i, \hat{c}_j\} = 2\delta_{ij}\hat{\mathbb{1}}.\tag{3.4}$$

Mathematically, these are the relations that define a *Clifford Algebra* (\mathcal{C}_{2N}). Moreover, the Majorana's operator are hermitian, as can be easily checked from the definition. Taking arbitrary complex linear combinations and products of these operators, including the identity, a generic element of this algebra can be written as

$$\hat{X} = \alpha\hat{\mathbb{1}} + \sum_{p=1}^{2n} \sum_{1 \leq i_1 < \dots < i_p \leq 2N} \alpha_{i_1, \dots, i_p} \hat{c}_{i_1} \cdots \hat{c}_{i_p}.\tag{3.5}$$

In particular, if we are interested in quadratic (free) Hamiltonians in the creation/annihilation operators, they can be parametrized by a real $2N \times 2N$ antisymmetric matrix H such that

$$\hat{H} = i \sum_{ij}^{2N} H_{ij} \hat{c}_j \hat{c}_i,\tag{3.6}$$

in order to fulfil hermiticity.

With the formalism we will develop, we will be able to treat pure and mixed fermionic states in the same way. We know that a generic state can be described by a density matrix that, by definition, is a hermitian and positive operator on the Hilbert space with trace one. If we consider fermionic systems, our Hilbert space is the Fock space of fermions $\mathcal{F}(N)$ with basis (3.2); a linear operator acting in this space can be written in terms of creation and annihilation operators or, equivalently, of Majorana's operators. So, for example, the density matrix $\rho = |0\rangle\langle 0|$ is represented in the operator's Algebra as

$$|0\rangle\langle 0| \mapsto \prod_{i=1}^N \hat{a}_i \hat{a}_i^\dagger = \frac{1}{2^N} \prod_{i=1}^N (\mathbb{1} + i\hat{c}_{2i-1} \hat{c}_{2i}).\tag{3.7}$$

It is straightforward to prove that the action of the left and right hand sides on the Fock basis is the same. Instead, the density matrix of a state with one particle in the first mode

is represented by

$$|1_1, 0_2, \dots, 0_N\rangle\langle 1_1, 0_2, \dots, 0_N| \mapsto \hat{a}_1^\dagger \hat{a}_1 \prod_{i=2}^N \hat{a}_i \hat{a}_i^\dagger = \frac{1}{2^N} (\mathbb{1} - i\hat{c}_1 \hat{c}_2) \prod_{i=2}^N (\mathbb{1} + i\hat{c}_{2i-1} \hat{c}_{2i}). \quad (3.8)$$

It is convenient to define a Grassmann variable **(B)** for each operator in the Clifford Algebra. Given $\hat{X} \in \mathcal{C}_{2N}$, we associate an element $X(\theta) \in \mathcal{G}_{2N}$ by the following rules:

$$\begin{aligned} \hat{X} = \mathbb{1} &\mapsto X(\theta) = 1, \\ \hat{X} = \hat{c}_{i_1} \hat{c}_{i_2} \cdots \hat{c}_{i_r} &\mapsto X(\theta) = \theta_{i_1} \theta_{i_2} \cdots \theta_{i_r}. \end{aligned} \quad (3.9)$$

This definition is extended by linearity to a generic element of \mathcal{C}_{2N} . We notice that this correspondence, that we call *Grassmann representation*, is just an isomorphism between vectorial spaces and not between algebras, since in general

$$\hat{X}\hat{Y} \not\mapsto X(\theta)Y(\theta) \quad (3.10)$$

due to the different anticommutation relations $\{\hat{c}_i, \hat{c}_j\} = 2\delta_{ij}\hat{\mathbb{1}}$ and $\{\theta_a, \theta_b\} = 0$.

For example, the operator $\hat{a}_1 \hat{a}_1^\dagger$ in terms of Majorana's operator is

$$\hat{X} = \hat{a}_1 \hat{a}_1^\dagger = \frac{1}{2} (\mathbb{1} + i\hat{c}_1 \hat{c}_2), \quad (3.11)$$

that in the Grassmann representation becomes

$$X(\theta) = \frac{1}{2} (1 + i\theta_1 \theta_2) = \frac{1}{2} e^{i\theta_1 \theta_2}, \quad (3.12)$$

where the exponential is defined by the Taylor series.

In the following we will extensively use a convenient formula to compute the trace of the product of two operators in the Clifford Algebra. It can be proven that the following relation holds:

$$\text{Tr}(\hat{X}\hat{Y}) = (-2)^N \int D\theta D\mu e^{\theta^T \mu} X(\theta) Y(\mu). \quad (3.13)$$

This formula is one of the main reason why we have introduced the Grassmann formalism for fermionic systems: it turns out that the integral above is easily computable in the case of gaussian operators (that are still to be defined) using the gaussian integrations **(B.8)** and **(B.9)**.

3.1.2 Construction of FPEPS

We now proceed with the construction of FPEPS following the fiducial state approach we used for PEPS. Differently from **3.1.1**, we consider now a system of fermions in the 2D lattice where the role of the previous N modes is now played by the N sites of the lattice: the n_r 's in **(3.2)** refer now to the number of fermions (again 0 or 1) that occupy the site r ($r = (x, y)$). The fermionic operators are now indexed by r : \hat{a}_r and \hat{a}_r^\dagger . In this picture we enable only one physical fermion per site, but we could generalize introducing χ physical

fermionic modes for each site: then, we should add an index $m = 1, \dots, f$ to the fermionic operators (\hat{a}_r^m and $\hat{a}_r^{m\dagger}$) and extend the anticommutation relations properly.

The fiducial state construction involves the introduction of a virtual layer. Precisely, we add two virtual fermionic operators to each site, one called horizontal, the other vertical: $\hat{h}_r, \hat{h}_r^\dagger, \hat{v}_r$ and \hat{v}_r^\dagger , satisfying again the anticommutation relations. Operators of different types always anticommute. From all these operators, one can construct the complete physical+virtual Fock space ($\mathcal{F}_{pv}(N)$) that has $\dim \mathcal{F}_{pv}(N) = 2^{3N}$. Throughout this chapter we will concentrate on the simplest FPEPS, those which have the smallest possible bond dimension. However all the construction given here can be easily generalize to larger bond dimension, starting by adding an index $n = 1, \dots, \chi$ to the fermionic operators ($\hat{h}_r^n, \hat{h}_r^{n\dagger}, \hat{v}_r^n$ and $\hat{v}_r^{n\dagger}$) and extending the anticommutation relations properly.

As done for generic fermionic systems, we change now formalism defining $6N$ Majorana's operators in the following way:

$$\begin{aligned}\hat{c}_r^1 &:= \hat{a}_r^\dagger + \hat{a}_r, \\ \hat{c}_r^2 &:= -i(\hat{a}_r^\dagger - \hat{a}_r), \\ \hat{\gamma}_r^l &:= \hat{h}_r^\dagger + \hat{h}_r, \\ \hat{\gamma}_r^r &:= -i(\hat{h}_r^\dagger - \hat{h}_r), \\ \hat{\gamma}_r^u &:= \hat{v}_r^\dagger + \hat{v}_r, \\ \hat{\gamma}_r^d &:= -i(\hat{v}_r^\dagger - \hat{v}_r),\end{aligned}\tag{3.14}$$

where the subscripts of the virtual operators stay for $l = \text{left}$, $r = \text{right}$, $u = \text{up}$ and $d = \text{down}$. These operators satisfy the Clifford algebra relations

$$\{\hat{m}_r^A, \hat{m}_s^{B\dagger}\} = 2\delta_{rs}\delta^{AB},\tag{3.15}$$

where \hat{m}_r^A stays for a generic Majorana operator (either physical or virtual) on the site r with appropriate index A corresponding to the selected mode.

The fiducial state construction starts from a physical+virtual operator assigned to each site and acting on the vacuum of the whole Fock space. Such a generic operator is written as

$$\phi_r^\dagger := \sum_{a,\alpha,\beta=0}^1 M_{\alpha\beta}^a \hat{a}_r^{a\dagger} \hat{h}_r^{\alpha\dagger} \hat{v}_r^{\beta\dagger},\tag{3.16}$$

where $M_{\alpha\beta}^a$ is a complex number. Applying these N operators on the vacuum $|0\rangle$ of $\mathcal{F}_{pv}(N)$, we obtain the total fiducial state $|\Phi\rangle$:

$$|\Phi\rangle := \prod_r \phi_r^\dagger |0\rangle^1.\tag{3.17}$$

The next step in the fiducial state construction involves the projections for each bond: in particular, for an horizontal bond between sites r and $r + \hat{x}$ we define

$$\hat{\omega}_r^h := \frac{1}{2}(\mathbb{1} - i\hat{\gamma}_{r+\hat{x}}^l \hat{\gamma}_r^r),\tag{3.18}$$

¹We notice that in the fermionic case is not possible to follow strictly the construction given in 2.2.1 because the tensor product between Fock fermionic states is not defined.

while for a vertical bond between r and $r + \hat{y}$

$$\hat{\omega}_r^v := \frac{1}{2}(\mathbb{1} - i\hat{\gamma}_{r+\hat{y}}^u \hat{\gamma}_r^d). \quad (3.19)$$

Conventionally we consider a reference frame from left to right and from up to down. The $\hat{\omega}$'s defined above are actually projectors, since $\hat{\omega}^2 = \hat{\omega}$ and $\hat{\omega}^\dagger = \hat{\omega}$, and commute with each other. After applying the total projector

$$\hat{\Omega} = \prod_r \hat{\omega}_r^h \hat{\omega}_r^v \quad (3.20)$$

to the total fiducial state $|\Phi\rangle$, the final FPEPS is obtained tracing out the virtual space (we neglect normalizations):

$$\begin{aligned} \rho &= \text{Tr}_V(\hat{\Omega}|\Phi\rangle\langle\Phi|\hat{\Omega}) \\ &= \text{Tr}_V(\hat{\Omega}|\Phi\rangle\langle\Phi|). \end{aligned} \quad (3.21)$$

The final step above is not due to the cyclicity of the trace, that in general does not hold for partial traces, but it can be proven remembering that $\hat{\Omega}$ is a projector.²

3.2 GFPEPS

3.2.1 Gaussian States

We define now an important class of states, the gaussian ones. The most important feature for gaussian state is that all their information is stored in the two point correlation matrix: we now see how to treat define and deal with them properly. We remember that a density matrix that represents a state in the Fock space can be written in terms of Majorana's operators as in subsection 3.1.1. Then, we give the following definition for a Gaussian state [4] from the Grassmann Algebra representation.

²We notice that the partial trace for fermionic systems of multiple modes is not a trivial object. In principle, one should take a basis for the subspace to be traced out, but this is not possible for fermions because the Fock space cannot be decomposed in a tensor product of each mode. Actually, this is not a problem [7]: we can define the partial trace treating formally the basis elements $|n_1, \dots, n_N\rangle$ as a tensor product $|n_1\rangle \otimes \dots \otimes |n_N\rangle$; the procedure to trace out some modes is then identical to the one for spins, except for possible ambiguities in the sign. Nevertheless, these ambiguities are completely resolved if we impose that a simple physical requirement, namely

$$\langle\mathcal{O}(A)\rangle_\rho = \langle\mathcal{O}(A)\rangle_{\text{Tr}_B(\rho)} \quad (3.22)$$

for every observable $\mathcal{O}(A)$ that is made by fermionic operators of the subsystem A ; B is the complementary subsystem. The result is proven to be consistent.

Let's give a simple example with two fermions; the basis vectors are $|0_1, 0_2\rangle$, $|1_1, 0_2\rangle$, $|0_1, 1_2\rangle$ and $|1_1, 1_2\rangle$. The partial trace over the second system is consistent with the above condition if we impose

$$\begin{aligned} \text{Tr}_2(|0_1, 0_2\rangle\langle 0_1, 0_2|) &= |0_1\rangle\langle 0_1|, & \text{Tr}_2(|0_1, 0_2\rangle\langle 0_1, 1_2|) &= 0, \\ \text{Tr}_2(|0_1, 0_2\rangle\langle 1_1, 0_2|) &= |0_1\rangle\langle 1_1|, & \text{Tr}_2(|0_1, 0_2\rangle\langle 1_1, 1_2|) &= 0, \\ \text{Tr}_2(|0_1, 1_2\rangle\langle 0_1, 1_2|) &= |0_1\rangle\langle 0_1|, & \text{Tr}_2(|0_1, 1_2\rangle\langle 1_1, 0_2|) &= 0, \\ \text{Tr}_2(|0_1, 1_2\rangle\langle 1_1, 1_2|) &= |0_1\rangle\langle 1_1|, & \text{Tr}_2(|1_1, 0_2\rangle\langle 1_1, 0_2|) &= |1_1\rangle\langle 1_1|, \\ \text{Tr}_2(|1_1, 0_2\rangle\langle 1_1, 1_2|) &= 0, & \text{Tr}_2(|1_1, 1_2\rangle\langle 1_1, 1_2|) &= |1_1\rangle\langle 1_1|. \end{aligned}$$

Definition (Gaussian state). A quantum state of N fermionic modes is *gaussian* if and only if its density matrix $\rho \in \mathcal{C}_{2N}$ has a Gaussian representation in the exponential form

$$\rho(\theta) = \frac{1}{2^N} e^{\frac{i}{2}\theta^T M \theta} \quad (3.23)$$

for some real and antisymmetric matrix M $2N \times 2N$. M is called *correlation matrix* of ρ .

The correlation matrix can be compute directly from the state ρ by the following formula:

$$M_{ij} = \frac{i}{2} \text{Tr}(\rho[\hat{c}_i, \hat{c}_j]) = \begin{cases} i \text{Tr}(\rho \hat{c}_i \hat{c}_j) & i \neq j \\ 0 & i = j \end{cases}. \quad (3.24)$$

To prove the above relation we can use the formula (3.13) to compute the trace in the the Clifford Algebra. Let's consider $i < j$ without loss of generality since M is antisymmetric:

$$i \text{Tr}(\rho \hat{c}_i \hat{c}_j) = i(-2)^N \int D\theta D\mu e^{\theta^T \mu} \rho(\theta)(c_i c_j)(\mu). \quad (3.25)$$

From (3.23) we rewrite $\rho(\theta)$ and we substitute the Majorana operators with the Grassmann variables:

$$i(-1)^N \int D\theta D\mu e^{\theta^T \mu} e^{\frac{i}{2}\theta^T M \theta} \mu_i \mu_j. \quad (3.26)$$

Since even polynomial of Grassmann variables commute with all the algebra, we can organize the integration in a convenient way:

$$i(-1)^N \int D\theta e^{\frac{i}{2}\theta^T M \theta} \int D\mu e^{\theta^T \mu} \mu_i \mu_j. \quad (3.27)$$

We rewrite the second exponential by the Taylor series, noticing that the series contains up to $2N$ terms, since the next terms would contain at least one variable twice and then would annihilate.

$$i(-1)^N \int D\theta e^{\frac{i}{2}\theta^T M \theta} \int D\mu \sum_{n=0}^{2N} \frac{(\theta^T \mu)^n}{n!} \mu_i \mu_j. \quad (3.28)$$

Using now the multinomial formula for commuting variables³, i.e. the quadratic terms in $\theta^T \mu$, we can study the integral more explicitly:

$$i(-1)^N \int D\theta e^{\frac{i}{2}\theta^T M \theta} \int D\mu \sum_{n=0}^{2N} \sum_{\substack{|\mathbf{k}|=n \\ k_l \in \{0,1\}}} \prod_{l=1}^{2N} (\theta_l \mu_l)^{k_l} \mu_i \mu_j. \quad (3.30)$$

³The multinomial formula is an extension of the binomial formula for a generic polynomial: suppose we have r commuting variables x_r , the multinomial formula gives

$$\left(\sum_{i=1}^r x_i \right)^n = \sum_{|\mathbf{k}|=n} \binom{n}{\mathbf{k}} \prod_{i=1}^r x_i^{k_i}, \quad (3.29)$$

where $\mathbf{k} = (k_1, \dots, k_r) \in \mathbb{N}^r$, $|\mathbf{k}| := \sum_{i=1}^r k_i$, $\binom{n}{\mathbf{k}} := \frac{n!}{\prod_{i=1}^r k_i!}$ (multinomial coefficient) and the sum is made over all possible choices of \mathbf{k} with the constraint $|\mathbf{k}| = n$. In our case with Grassmann variables, this formula simplifies: we note that k_i 's can only take the values 0 or 1, otherwise $(\theta_j \mu_j)^{k_i \geq 2} = 0$; in this case, also the multinomial coefficient simplifies and for every \mathbf{k} we have $\binom{n}{\mathbf{k}} := n!$.

Since the integration in $D\mu$ requires that each μ_l appears exactly once, otherwise annihilates, we can keep only the terms with $n = 2N - 2$, $k_l = 1$ for $l \neq i, j$ and $k_i = k_j = 0$:

$$i(-1)^N \int D\theta e^{\frac{i}{2}\theta^T M \theta} \int D\mu \left(\prod_{\substack{l=1 \\ l \neq i, j}}^{2N} \theta_l \mu_l \right) \mu_i \mu_j. \quad (3.31)$$

We skip now the detailed proof, only proving that the above expression is equal to M_{ij} except for a possible sign that one can rigorously calculate, finding $+$. Neglecting the sign, the integration over $D\mu$ then gives:

$$i \int D\theta e^{\frac{i}{2}\theta^T M \theta} \left(\prod_{\substack{l=1 \\ l \neq i, j}}^{2N} \theta_l \right). \quad (3.32)$$

We should now expand the exponential in the Taylor series: however, the only terms in the sum that do not give a null contribution to the integral in $D\theta$ are the ones that contains only θ_i and θ_j , namely the terms $\frac{i}{2}\theta_i M_{ij} \theta_j$ and $\frac{i}{2}\theta_j M_{ji} \theta_i$. Skipping again the sign, after the integration we obtain

$$\left(\frac{1}{2} M_{ij} - \frac{1}{2} M_{ji} \right) = M_{ij}, \quad (3.33)$$

as we wanted to prove.

We know that a gaussian state is completely described by the correlation matrix. Indeed, all higher correlations are determined by the Wick formula, namely

$$i^p \text{Tr}(\rho \hat{c}_{i_1} \cdots \hat{c}_{i_p}) = \text{Pf}(M|_{a_1, \dots, a_{2p}}),$$

with $1 \leq a_1 < \dots < a_{2p} \leq 2n$ and $M|_{a_1, \dots, a_{2p}}$ the $2p \times 2p$ submatrix with the indicated rows and columns.

Is is known that any real $2N \times 2N$ antisymmetric matrix M can be transformed into a block-diagonal form by an orthogonal change of basis, with all the blocks being 2×2 antisymmetric matrices:

$$M = R \bigoplus_{i=1}^N \begin{pmatrix} 0 & \lambda_i \\ -\lambda_i & 0 \end{pmatrix} R^T, \quad R \in SO(2N), \quad (3.34)$$

where λ_i are real numbers. In the new basis, we can rewrite our gaussian state ρ expanding the exponential in (3.23) and reintroducing the Majorana's operators, obtaining a canonical product form

$$\rho(\lambda_1, \dots, \lambda_N) = \frac{1}{2^N} \prod_{i=1}^N (\mathbb{1} + i\lambda_i \hat{c}'_{2i-1} \hat{c}'_{2i}), \quad (3.35)$$

where the new Majorana's operators are linear combinations of the initial ones: $\hat{c}'_i = \sum_j^{2N} R_{ji} \hat{c}_j$. The anticommutation relations still hold since the change of basis R is orthogonal⁴. With ρ in this form, the non negativity of the density matrix is equivalent to having

$$-1 \leq \lambda_i \leq 1, \quad \forall i = 1, \dots, N, \quad (3.36)$$

as one prove taking each basis vector $|\psi\rangle$ from (3.2) and imposing $\langle \psi | \rho | \psi \rangle \geq 0$. In terms of the correlation matrix M , this condition reads

$$M^T M \leq \mathbb{1}, \quad (3.37)$$

valid regardless of the change of basis. Together with antisymmetry, this condition is necessary and sufficient for a matrix M to be a correlation matrix of some fermionic state. If the state ρ is pure, the coefficients λ_i must be $= \pm 1$ in order to satisfy $\rho = \rho^2$ and $\text{Tr}(\rho) = 1$, then the relation above for the correlation matrix reads

$$M^T M = \mathbb{1}, \quad (3.38)$$

or, equivalently, $M^2 = -\mathbb{1}$ due to the antisymmetry of M .

Translational invariant gaussian state on a lattice

We restrict ourself to the case of translational invariant gaussian states on a lattice with periodic boundary condition: to be consistent with the other section, we can think of a 2-dimensional lattice, but here the discussion is totally valid also in other dimensions. As in our previous conventions, the Majorana's operators are $\{\hat{c}_r^a\}$, with r the index of the lattice site and a an index going from 1 to $2f$, with f the number of fermionic modes that we allow in one site (usually for us $f = 1$). In terms of the correlation matrix, the condition of translational invariant imposes

$$G_{r+R, s+R}^{ab} = G_{r, s}^{ab}, \quad (3.39)$$

where $G_{r, s}^{ab} := \frac{i}{2} \text{Tr}(\rho[\hat{c}_r^a, \hat{c}_s^b])$.

To take advantage of this property, firstly we decompose the physical Majorana's operators in Fourier components:

$$\begin{aligned} \hat{c}_r^a &= \sum_k \mathcal{F}_{rk} \hat{d}_k^a = \sum_k \mathcal{F}_{rk}^* \hat{d}_k^{a\dagger}, \\ \hat{d}_k^a &:= \sum_r \mathcal{F}_{rk}^* \hat{c}_r^a, \\ \hat{d}_k^{a\dagger} &:= \sum_r \mathcal{F}_{rk} \hat{c}_r^a, \end{aligned} \quad (3.40)$$

⁴ $\{\hat{c}'_i, \hat{c}'_j\} = \{\hat{c}_k, \hat{c}_l\} R_{ki} R_{lj} = 2\delta_{kl} R_{ki} R_{lj} = 2R_{ki} R_{kj} = 2\delta_{ij}$.

where

$$\begin{aligned}\mathcal{F}_{rk}^{ab} &:= \delta^{ab} \mathcal{F}_{rk}, \\ \mathcal{F}_{rk} &:= \frac{1}{\sqrt{N}} e^{ir \cdot k}.\end{aligned}\tag{3.41}$$

The momenta k are quantized: calling N_x the number of sites per row and N_y the number site per column ($N = N_x N_y$), we have

$$k = (k_x, k_y) = \left(\frac{2\pi n_x}{N_x}, \frac{2\pi n_y}{N_y} \right),\tag{3.42}$$

with $n_x = 1, \dots, N_x$ and $n_y = 1, \dots, N_y$. The \mathcal{F} matrix is then unitary

$$\mathcal{F}\mathcal{F}^\dagger = \mathcal{F}^\dagger\mathcal{F} = \mathbb{1},\tag{3.43}$$

either if we consider \mathcal{F} with only lower indexes ($\sum_r \mathcal{F}_{rk} \mathcal{F}_{rp}^* = \delta_{kp}$ and $\sum_k \mathcal{F}_{rk} \mathcal{F}_{sk}^* = \delta_{rs}$) or we take the tensor product between lower and upper indexes ($\sum_{r,b} \mathcal{F}_{rk}^{ab} \mathcal{F}_{rp}^{bc*} = \delta^{ac} \delta_{kp}$ and $\sum_{k,b} \mathcal{F}_{rk}^{ab} \mathcal{F}_{sk}^{bc*} = \delta^{ac} \delta_{rs}$).

The new operators \hat{d}_k^a and $\hat{d}_k^{a\dagger}$ are the hermitian conjugate of the other and in general are different, so they cannot be Majorana's operators (the only exception is $\hat{d}_0^a = \hat{d}_0^{a\dagger}$). Instead, we have that $\hat{d}_k^a = \hat{d}_{-k}^{a\dagger}$. These \hat{d} s operators satisfy the following anticommutation relations:

$$\begin{aligned}\{\hat{d}_k^a, \hat{d}_p^{b\dagger}\} &= 2\delta^{ab} \delta_{kp} \hat{\mathbb{1}}, \\ \{\hat{d}_k^a, \hat{d}_p^b\} &= 2\delta^{ab} \delta_{k+p,0} \hat{\mathbb{1}}, \\ \{\hat{d}_k^{a\dagger}, \hat{d}_p^{b\dagger}\} &= 2\delta^{ab} \delta_{k+p,0} \hat{\mathbb{1}}.\end{aligned}\tag{3.44}$$

If now we defined a new correlation matrix \tilde{G} that involves the new \hat{d} s operators in the following way

$$\tilde{G}_{kp}^{ab} := \frac{i}{2} \text{Tr}(\rho[\hat{d}_k^a, \hat{d}_p^{b\dagger}]),\tag{3.45}$$

it is easy to see that G and \tilde{G} are connected by the orthogonal matrix \mathcal{F} :

$$G = \mathcal{F}\tilde{G}\mathcal{F}^\dagger.\tag{3.46}$$

Again, the above equation holds either we consider only lower indexes contraction with fixed upper indexes ($G_{rs}^{ab} = \sum_{k,p} \mathcal{F}_{rk} \tilde{G}_{kp}^{ab} \mathcal{F}_{sp}^*$) or we consider the bigger \mathcal{F} and contract also over the upper indexes ($G_{rs}^{ab} = \sum_{k,p,c,d} \mathcal{F}_{rk}^{ac} \tilde{G}_{kp}^{cd} \mathcal{F}_{sp}^{bd*}$).

Using the translational invariance (3.39), we can see what happen to the new correlation matrix \tilde{G} :

$$\begin{aligned}\tilde{G}_{kp}^{ab} &= \sum_{r,s} \mathcal{F}_{rk}^* G_{rs}^{ab} \mathcal{F}_{sp} \\ &= \sum_{r,s} \mathcal{F}_{rk}^* G_{r-s+R,R}^{ab} \mathcal{F}_{sp}.\end{aligned}\tag{3.47}$$

If we call $t := s - r$ and sum over r and t (thanks to the periodic boundary conditions) we get

$$\begin{aligned}
\tilde{G}_{kp}^{ab} &= \sum_{r,t} \mathcal{F}_{rk}^* G_{t+R,R}^{ab} \mathcal{F}_{t+r,p} \\
&= \sum_{r,t} \mathcal{F}_{r,k-p}^* G_{t+R,R}^{ab} \mathcal{F}_{t,p} \\
&= \delta_{k,p} \sqrt{N} \sum_t G_{t+R,R}^{ab} \mathcal{F}_{t,p} \\
&= \delta_{k,p} \sum_t G_{t+R,R}^{ab} e^{ip \cdot t}.
\end{aligned} \tag{3.48}$$

We define now

$$g^{ab}(k) := \sum_t G_{t+R,R}^{ab} e^{ik \cdot t} \tag{3.49}$$

for a generic R thanks to translational invariance. $g(k)$ is a matrix 2×2 defined for every momentum k . Then \tilde{G} is a block diagonal matrix with blocks given by $g(k)$:

$$\tilde{G} = \bigoplus_k g(k). \tag{3.50}$$

From the properties of antisymmetry, reality and orthogonality of the matrix G

$$G^T = -G, \quad G^* = G, \quad G^T G = \mathbb{1}, \tag{3.51}$$

we can obtain some general constraints for $g(k)$. From the antisymmetry:

$$\tilde{G}^\dagger = \mathcal{F}^\dagger G^T \mathcal{F} = -\mathcal{F}^\dagger G \mathcal{F} = -\tilde{G}, \tag{3.52}$$

from reality:

$$\tilde{G}_{kp}^* = (\mathcal{F}^\dagger G \mathcal{F})_{kp}^* = \sum_{rs} \mathcal{F}_{rk} G_{rs} \mathcal{F}_{sp}^* = \sum_{rs} \mathcal{F}_{r,-k}^* G_{rs} \mathcal{F}_{s,-p} = \tilde{G}_{-k,-p}, \tag{3.53}$$

while from orthogonality:

$$\tilde{G}^\dagger \tilde{G} = \mathcal{F}^\dagger G^T \mathcal{F} \mathcal{F}^\dagger G \mathcal{F} = \mathcal{F}^\dagger G^T G \mathcal{F} = \mathcal{F}^\dagger \mathbb{1} \mathcal{F} = \mathbb{1}. \tag{3.54}$$

For $g(k)$ the above relations reads

$$g(k)^\dagger = -g(k), \quad g(k)^* = g(-k), \quad g(k)^\dagger g(k) = \mathbb{1}. \tag{3.55}$$

The antihermiticity allows us to parametrize $g(k)$ in a convenient way when they are only 2×2 , i.e. when our system allow only one physical fermion per site ($f = 1$). Since the Pauli matrices (including the identity $\sigma_0 = \mathbb{1}_{2 \times 2}$) are hermitian matrices, $i\sigma_\mu$ are antihermitian and form a real basis for all antihermitian matrices; then we can generically write

$$g(k) = \begin{pmatrix} i(g^0(k) + g^3(k)) & g^2(k) + ig^1(k) \\ -g^2(k) + ig^1(k) & i(g^0(k) - g^3(k)) \end{pmatrix} = ig^\mu(k) \sigma_\mu, \tag{3.56}$$

where $g^\mu(k)$ are real components and can be found from

$$g^\mu(k) = -\frac{i}{2}\text{tr}(g(k)\sigma_\mu). \quad (3.57)$$

From orthogonality we find

$$\begin{aligned} \mathbb{1} &= g^\dagger g = \sum_{\mu,\nu=0}^3 g^\mu g^\nu \sigma_\mu \sigma_\nu \\ &= g^0 g^0 \sigma_0 \sigma_0 + \sum_{i=1}^3 g^0 g^i \sigma_0 \sigma_i + \sum_{i=1}^3 g^i g^0 \sigma_i \sigma_0 + \sum_{i,j=1}^3 g^i g^j \sigma_i \sigma_j \\ &= g^0 g^0 \mathbb{1} + 2 \sum_{i=1}^3 g^0 g^i \sigma_i + \sum_{i,j=1}^3 g^i g^j \left(i \sum_{k=1}^3 \epsilon_{ijk} \sigma_k + \delta_{ij} \mathbb{1} \right) \\ &= g^0 g^0 \mathbb{1} + 2 \sum_{i=1}^3 g^0 g^i \sigma_i + \sum_{i=1}^3 g^i g^i \mathbb{1}. \end{aligned} \quad (3.58)$$

We can see that to satisfy orthogonality, for each k either we have $g^i(k) = 0 \forall i$ and $g^0(k) = \pm 1$ or $g^0(k) = 0$ and $\sum_i g^i(k)^2 = 1$.

Ground states of two-bands Hamiltonians

Given a quadratic and translational invariant two-bands Hamiltonian

$$\hat{H} = i \sum_{rs} \sum_{ab}^2 H_{rs}^{ab} \hat{c}_s^b \hat{c}_r^a, \quad (3.59)$$

with H real and antisymmetric and $a, b = 1, 2$, we try to find its ground state by minimizing its energy. First we rewrite \hat{H} in terms of the Fourier transformed operators \hat{d}_s :

$$\hat{H} = i \sum_{kp} \sum_{ab}^2 \tilde{H}_{kp}^{ab} \hat{d}_p^b \hat{d}_k^{a\dagger}, \quad (3.60)$$

where the matrix of the coefficients \tilde{H} is given by

$$\tilde{H} = \mathcal{F}^\dagger H \mathcal{F}, \quad (3.61)$$

in complete analogy with the correlation matrix of a gaussian state. Furthermore, if \hat{H} is translational invariant we can obtain the coefficients in terms of a 2×2 matrix $h(k)$ that depend only on one momentum:

$$\tilde{H} = \bigoplus_k h(k). \quad (3.62)$$

From the antisymmetry and reality of H we obtain the following constraints for $h(k)$:

$$h(k)^\dagger = -h(k), \quad h(k)^* = h(-k). \quad (3.63)$$

Then, also $h(k)$ can be written as a linear combination of Pauli matrices:

$$h(k) = \begin{pmatrix} i(h^0(k) + h^3(k)) & h^2(k) + ih^1(k) \\ -h^2(k) + ih^1(k) & i(h^0(k) - h^3(k)) \end{pmatrix} = ih^\mu(k)\sigma_\mu, \quad (3.64)$$

with $h^\mu(k)$ real.

Given $h(k)$, we try now to minimize the energy over fermionic states ρ :

$$\text{Tr}(\hat{H}\rho) = i \sum_{kp} \sum_{ab} \tilde{H}_{kp}^{ab} \text{Tr}(\hat{d}_p^b \hat{d}_k^{a\dagger} \rho) = \frac{i}{2} \sum_{kp} \sum_{ab} \tilde{H}_{kp}^{ab} \text{Tr}([\hat{d}_p^b, \hat{d}_k^{a\dagger}] \rho). \quad (3.65)$$

We show the validity of the second equality:

$$\begin{aligned} \frac{i}{2} \sum_{kp} \sum_{ab} \tilde{H}_{kp}^{ab} \text{Tr}([\hat{d}_p^b, \hat{d}_k^{a\dagger}] \rho) &= \frac{i}{2} \sum_{kp} \sum_{ab} \tilde{H}_{kp}^{ab} \text{Tr}(\hat{d}_p^b \hat{d}_k^{a\dagger} \rho) - \frac{i}{2} \sum_{kp} \sum_{ab} \tilde{H}_{kp}^{ab} \text{Tr}(\hat{d}_k^{a\dagger} \hat{d}_p^b \rho) \\ &= i \sum_{kp} \sum_{ab} \tilde{H}_{kp}^{ab} \text{Tr}(\hat{d}_p^b \hat{d}_k^{a\dagger} \rho) - \frac{i}{2} \sum_{kp} \sum_{ab} \tilde{H}_{kp}^{ab} \text{Tr}(\{\hat{d}_k^{a\dagger}, \hat{d}_p^b\} \rho) \\ &= i \sum_{kp} \sum_{ab} \tilde{H}_{kp}^{ab} \text{Tr}(\hat{d}_p^b \hat{d}_k^{a\dagger} \rho) - \frac{i}{2} \sum_k \sum_a \tilde{H}_{kk}^{aa} \text{Tr}(\rho) \\ &= i \sum_{kp} \sum_{ab} \tilde{H}_{kp}^{ab} \text{Tr}(\hat{d}_p^b \hat{d}_k^{a\dagger} \rho), \end{aligned} \quad (3.66)$$

since

$$\sum_k \sum_a \tilde{H}_{kk}^{aa} = \text{tr}(\tilde{H}) = \sum_k \text{tr}(h(k)) = \text{tr}(h(0)) + \sum_{k>0} (\text{tr}(h(k)) + \text{tr}(h(-k))) = 0 \quad (3.67)$$

from (3.63). Proceeding with (3.65), we notice that we can substitute part of the expression with the correlation matrix of ρ :

$$\text{Tr}(\hat{H}\rho) = \sum_{kp} \sum_{ab} \tilde{H}_{kp}^{ab} \tilde{G}_{pk}^{ba} = \text{tr}(\tilde{H}\tilde{G}) = \sum_k \text{tr}(h(k)g(k)). \quad (3.68)$$

The minimization problem then reduces to find the matrices $g(k)$ that minimizes independently each term in the sum, with the constraints (3.55). We reintroduce the real components of $g(k)$ and $h(k)$ and rewrite

$$\epsilon(k) := \text{tr}(h(k)g(k)) = - \sum_{\mu,\nu}^4 h^\mu(k) g^\nu(k) \text{tr}(\sigma_\mu \sigma_\nu) = -2 \sum_{\mu}^4 h^\mu(k) g^\mu(k). \quad (3.69)$$

We first study the case $g^0(k) = 0$ and $\sum_i^3 g^i(k) = 1$. We use the Lagrangian multiplier method, searching for the stationary points of $f(g) := -2 \sum_i^3 h^i g^i + \lambda(1 - \sum_i^3 g^i)$. The stationary point turns out to be $g^i = -\frac{h^i}{\lambda}$. Imposing the constraint $\sum_i^3 g^i(k) = 1$, we find the multiplier $\lambda = \pm \sqrt{\sum_i^3 h^i h^i}$. Choosing the negative solution, we get the coefficients of the ground state and the minimum energy:

$$\begin{aligned} g^i(k) &= \frac{h^i(k)}{\sqrt{\sum_j^3 h^j(k)h^j(k)}}, \\ \epsilon(k) = -\varepsilon(k) &= -2\sqrt{\sum_i^3 h^i(k)h^i(k)}. \end{aligned} \tag{3.70}$$

This solution should be compared with the case $g^i(k) = 0$ and $g^0(k) = \pm 1$. The computation of the energy with these constraints gives $\epsilon(k) = \mp 2h^0(k)$, to be compared with the above solution to find the point of minimum.

If $h^0(k) = 0 \forall k$, we have found that the correlation matrices $g(k)$ of the gaussian ground state are proportional to $h(k)$, the matrix of coefficients (in Fourier transform), for each k . In some sense also the inverse is true for 2-bands systems: given a gaussian state described by a 2×2 correlation matrix $g(k)$ with $g^0(k) = 0 \forall k$, all the translational invariant, quadratic parent Hamiltonians must have a matrix of coefficients in the form

$$h(k) = \frac{\epsilon(k)}{2} g(k), \tag{3.71}$$

with an arbitrary function $\epsilon(k) \geq 0$. The proof follows exactly the same steps above: in particular we want to find all the $h^i(k)$ s such that the minimum of

$$-2 \sum_i^3 h^i(k) g^i(k) \tag{3.72}$$

over the correlation matrix coefficients $g^i(k)$ is reached when $g^i(k) = g^i(k)$. But, as we have seen, to minimize the above expression we need $g^i(k) \propto h^i(k)$ with a proportionality constant independent on i , and then we find (3.71).

3.2.2 Construction of GFPEPS

We are ready now to treat gaussian fermionic PEPS. A *gaussian fermionic PEPS* is defined to be a FPEPS constructed from a gaussian fiducial state $|\phi_r\rangle := \hat{\phi}_r^\dagger |0\rangle$. As in subsection 3.1.2, we will consider the simplest case where we have one physical fermionic mode and two virtual fermionic modes allowed for each of the N sites. We now follow the fiducial state construction and find how we can simplify the analytical computations in the correlation matrices formalism.

The initial gaussian fiducial state is described by a correlation matrix M 6×6 ⁵. We organize this correlation matrix in four blocks, one corresponding to the correlations between physical modes (A , 2×2), an other with correlations between virtual modes (D , 4×4) and a third block corresponding to mixed correlations (B , 2×4):

$$\begin{aligned} M &= \begin{pmatrix} A & B \\ -B^T & D \end{pmatrix}, \\ A^{ab} &= \frac{i}{2} \text{Tr}(\rho_\phi[\hat{c}^a, \hat{c}^b]), \\ B^{a\beta} &= \frac{i}{2} \text{Tr}(\rho_\phi[\hat{c}^a, \hat{\gamma}^\beta]), \\ D^{\alpha\beta} &= \frac{i}{2} \text{Tr}(\rho_\phi[\hat{\gamma}^\alpha, \hat{\gamma}^\beta]), \end{aligned} \quad (3.73)$$

where $a, b = 1, 2$ and $\alpha, \beta = l, r, u, d$ (we neglect the subscript r of the site if not necessary); ρ_ϕ is the density matrix of $|\phi_r\rangle$: $\rho_\phi = |\phi_r\rangle\langle\phi_r|$. After the action of ϕ_r^\dagger on the vacuum for each site, the correlation matrix \mathcal{M} of the total fiducial state $|\Phi\rangle = \prod_r \phi_r^\dagger|0\rangle$ is given by the direct sum of the correlation matrices for each site:

$$\mathcal{M} = \bigoplus_r M = \begin{pmatrix} M & & \\ & \ddots & \\ & & M \end{pmatrix}. \quad (3.74)$$

Explicitly, this big matrix in terms of components is given by \mathcal{M}_{rs}^{AB} , where $A, B = 1, 2, l, r, u, d$ and r, s are the vectors that span the entire lattice of N sites. The matrix is then $6N \times 6N$. We call ρ_Φ the corresponding density matrix: $\rho_\Phi = |\Phi\rangle\langle\Phi|$. By a reshaping of the correlation matrix, we can write it in the four blocks form

$$\mathcal{M} = \begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B}^T & \mathcal{D} \end{pmatrix}, \quad (3.75)$$

where the blocks \mathcal{A} , \mathcal{B} and \mathcal{D} are given by the direct sum of A , B and D respectively.

The next step in the fiducial state construction involves the projection on entangled virtual modes by the operator $\hat{\Omega}$ defined in (3.20). Rewriting it in terms of Grassmann

⁵Strictly speaking, the state $\hat{\phi}_r^\dagger|0\rangle$ lives in the total Fock space $\mathcal{F}_{pv}(N)$ and then its correlation matrix should be $6N \times 6N$; however, since $\hat{\phi}_r^\dagger$ is an operator constructed only from creation and annihilation operators on the site r , the total correlation matrix $6N \times 6N$ is non trivial only at position r on the diagonal, where it is described by M . The rest is "trivial", meaning that the rest of the diagonal is composed by 2×2 blocks $\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ corresponding to the absence of particles for each site $\neq r$ and for each mode.

variables, we find

$$\begin{aligned}
\Omega(\mu) &= \prod_r \frac{1}{2} \left(1 - i\mu_{r+\hat{x}}^l \mu_r^r\right) \frac{1}{2} \left(1 - i\mu_{r+\hat{y}}^u \mu_r^d\right) = \\
&= \frac{1}{2^{2N}} \prod_r e^{-i\mu_{r+\hat{x}}^l \mu_r^r} e^{-i\mu_{r+\hat{y}}^u \mu_r^d} = \\
&= \frac{1}{2^{2N}} e^{-i \sum_r (\mu_{r+\hat{x}}^l \mu_r^r + \mu_{r+\hat{y}}^u \mu_r^d)} \\
&=: \frac{1}{2^{2N}} e^{\frac{i}{2} \mu^T \Gamma \mu}.
\end{aligned} \tag{3.76}$$

We conclude that our projector $\hat{\Omega}$ actually can represent a gaussian state. This state corresponds exactly to the initial virtual state (2.15) in the valence bond construction of PEPS. Its correlation matrix $\Gamma_{rr'}^{\alpha\alpha'}$ is given explicitly by

$$\begin{aligned}
\Gamma_{xyx'y'}^{\alpha\alpha'} &= -\delta_{x,x'+1} \delta_{y,y'} \delta^{\alpha,l} \delta^{\alpha',r} + \delta_{x+1,x'} \delta_{y,y'} \delta^{\alpha,r} \delta^{\alpha',l} \\
&\quad - \delta_{x,x'} \delta_{y,y'+1} \delta^{\alpha,u} \delta^{\alpha',d} + \delta_{x,x'} \delta_{y+1,y'} \delta^{\alpha,d} \delta^{\alpha',u}.
\end{aligned} \tag{3.77}$$

Furthermore it can be show that, as a gaussian state, $\hat{\Omega}$ is pure because $\Gamma^T \Gamma = \mathbb{1}$. To make the above correlation matrix more explicit, we consider only left and right Majorana operators on a horizontal line, say $x = 1$ (but the same holds for every row for translation invariance), with the ordering $\hat{\gamma}_{1,1}^l, \hat{\gamma}_{1,1}^r, \hat{\gamma}_{1,2}^l, \hat{\gamma}_{1,2}^r, \dots, \hat{\gamma}_{1,N_y}^l, \hat{\gamma}_{1,N_y}^r$. Then we can write a matrix Γ_h where the entries correspond to the correlations between the operator on the row and the operator on the column:

$$\Gamma_h = \begin{pmatrix} 0 & 0 & & & & & -1 \\ 0 & 0 & 1 & & & & \\ & -1 & 0 & 0 & & & \\ & & 0 & 0 & 1 & & \\ & & & -1 & \ddots & \ddots & \\ & & & & \ddots & 0 & 0 \\ 1 & & & & & 0 & 0 \end{pmatrix} \tag{3.78}$$

The 1s on the upper right and bottom left corners are due to the periodic boundary conditions. We could do the same for a vertical line and up and down Majorana operators, obtaining $\Gamma_v = \Gamma_h$.

To compute the final GFPEPS we should then use formula (3.21):

$$\rho = \text{Tr}_V(\hat{\Omega} \rho_\Phi). \tag{3.79}$$

Taking advantage of the gaussianity of the two operators inside the trace, we can do some calculations using the formula for the trace in the Clifford Algebra (3.13), slightly generalized to the case of partial trace. We use μ and ν to label Grassmann variables of

the virtual Majorana's operators and θ for the physical ones.

$$\begin{aligned}\rho(\theta) &= (-2)^{2N} \int D\mu D\nu e^{\mu^T \nu} \Omega(\mu) \rho_{\Phi}(\theta, \nu) = \\ &= (-2)^{2N} \int D\mu D\nu e^{\mu^T \nu} \frac{1}{2^{2N}} e^{\frac{i}{2} \mu^T \Gamma \mu} \frac{1}{2^{3N}} e^{\frac{i}{2} \mathcal{E}(\theta, \nu)},\end{aligned}\quad (3.80)$$

where

$$\mathcal{E}(\theta, \nu) = (\theta^T \nu^T) \mathcal{M} \begin{pmatrix} \theta \\ \nu \end{pmatrix} = \theta^T \mathcal{A} \theta + 2\theta^T \mathcal{B} \nu + \nu^T \mathcal{D} \nu. \quad (3.81)$$

We reorganize the integration, remembering that quadratic forms of Grassmann variables always commute with the Algebra:

$$\begin{aligned}\rho(\theta) &= \frac{1}{2^N} \int D\mu D\nu e^{\mu^T \nu + \frac{i}{2} \mu^T \Gamma \mu + \frac{i}{2} \theta^T \mathcal{A} \theta + i\theta^T \mathcal{B} \nu + \frac{i}{2} \nu^T \mathcal{D} \nu} = \\ &= \frac{1}{2^N} \int D\nu \left(\int D\mu e^{\nu^T \mu + \frac{i}{2} \mu^T \Gamma \mu} \right) e^{\frac{i}{2} \theta^T \mathcal{A} \theta + i\theta^T \mathcal{B} \nu + \frac{i}{2} \nu^T \mathcal{D} \nu}.\end{aligned}\quad (3.82)$$

Applying the gaussian integration formula (B.9), we get

$$\begin{aligned}\rho(\theta) &= \frac{i^2}{2^N} \text{Pf}(\Gamma) \int D\nu e^{-\frac{i}{2} \nu^T \Gamma^{-1} \nu + \frac{i}{2} \theta^T \mathcal{A} \theta + i\theta^T \mathcal{B} \nu + \frac{i}{2} \nu^T \mathcal{D} \nu} = \\ &= -\frac{1}{2^N} \text{Pf}(\Gamma) e^{\frac{i}{2} \theta^T \mathcal{A} \theta} \int D\nu e^{\frac{i}{2} \nu^T (\mathcal{D} - \Gamma^{-1}) \nu - i(\mathcal{B}^T \theta)^T \nu}.\end{aligned}\quad (3.83)$$

Finally, with the same gaussian integration formula used above, supposing that $\det(\mathcal{D} - \Gamma^{-1}) \neq 0$, we obtain

$$\begin{aligned}\rho(\theta) &= -\frac{i^2}{2^N} \text{Pf}(\Gamma) \text{Pf}(\mathcal{D} - \Gamma^{-1}) e^{\frac{i}{2} \theta^T \mathcal{A} \theta} e^{\frac{i}{2} (\mathcal{B}^T \theta)^T (\mathcal{D} - \Gamma^{-1})^{-1} (\mathcal{B}^T \theta)} = \\ &= \frac{1}{2^N} \text{Pf}(\Gamma) \text{Pf}(\mathcal{D} - \Gamma^{-1}) e^{\frac{i}{2} \theta^T (\mathcal{A} + \mathcal{B}(\mathcal{D} - \Gamma^{-1})^{-1} \mathcal{B}^T) \theta}.\end{aligned}\quad (3.84)$$

Remembering that $\Gamma^{-1} = -\Gamma$ because orthogonal and antisymmetric, we conclude that the GFPEPS is actually a gaussian state with correlation matrix G ($2N \times 2N$) given by

$$G = \mathcal{A} + \mathcal{B}(\mathcal{D} + \Gamma)^{-1} \mathcal{B}^T. \quad (3.85)$$

GFPEPS in Fourier transform

The formula above is useful to compute the correlation matrix of a generic GFPEPS: all the information of the state is contained in the matrix G . However, at first sight it seems that the above formula involves too big matrices (of the order $N \times N$) respect to the small number of parameters that compose them. It is not even clear how we should take the thermodynamic limit of the system without further increasing the dimension of such matrices. All these problems arise because we have not yet take advantage of the translation

invariance of the system. Indeed, the computation simplifies a lot if we go to momentum space by Fourier transform.

Our system is translational invariant by construction: we have built a generic GFPEPS starting from an individual fiducial state placed in each site and projecting in the same way all neighbouring sites. The projection includes also the first and the last site of each row and column, implementing in this way the periodic boundary conditions.

As in 3.2.1, the translational invariance permits the definitions

$$\begin{aligned}\mathcal{F}^\dagger \Gamma \mathcal{F} &=: \bigoplus_k \gamma(k), \\ \mathcal{F}^\dagger G \mathcal{F} &=: \bigoplus_k g(k),\end{aligned}\tag{3.86}$$

for both the correlation matrices of the gaussian virtual projector and the GFPEPS.

Here $\gamma(k)$ is then a matrix 4×4 . From the explicit expression of Γ in (3.77), we can find

$$\gamma(k) = \begin{pmatrix} 0 & e^{-ik_x} & 0 & 0 \\ -e^{ik_x} & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{-ik_y} \\ 0 & 0 & -e^{ik_y} & 0 \end{pmatrix}.\tag{3.87}$$

We proceed now in the computation of $g(k)$ starting from $\gamma(k)$ and the formula (3.85). Applying \mathcal{F}^\dagger to the left and \mathcal{F} to the right of equation (3.85), we obtain

$$\tilde{G} = \mathcal{F}^\dagger \mathcal{A} \mathcal{F} + \mathcal{F}^\dagger \mathcal{B} (\mathcal{D} + \Gamma)^{-1} \mathcal{B}^T \mathcal{F}.\tag{3.88}$$

We recall that the matrices \mathcal{A} , \mathcal{B} and \mathcal{D} are diagonal in space, so they commute with \mathcal{F} :

$$\tilde{G} = \mathcal{A} + \mathcal{B} (\mathcal{D} + \mathcal{F}^\dagger \Gamma \mathcal{F})^{-1} \mathcal{B}^T = \mathcal{A} + \mathcal{B} (\mathcal{D} + \tilde{\Gamma})^{-1} \mathcal{B}^T.\tag{3.89}$$

We have found a matrix expression involving only diagonal matrices, then we end up with

$$g(k) = A + B (D + \gamma(k))^{-1} B^T.\tag{3.90}$$

In summary, given a fiducial state described by the correlation matrices A , B and D , the above formula gives the correlation matrix $g(k)$ that describes completely the GFPEPS. To get more information about the formula above, we rewrite the inverse of the matrix in terms of the adjugate matrix⁶ and the determinant $q(k) := \det(D + \gamma(k))$:

$$g(k) = A + B \frac{\text{Adj}(D + \gamma(k))}{q(k)} B^T.\tag{3.93}$$

⁶The adjugate matrix of a matrix A is given by the matrix

$$\text{Adj}(A)_{ij} = (-i)^{i+j} \det A_{(j,i)}\tag{3.91}$$

where $A_{(j,i)}$ is the matrix formed by deleting the j -row and i -column of A . The following relation holds:

$$A \text{Adj}(A) = \det(A) \mathbb{1}\tag{3.92}$$

from which we can find the inverse of A in terms of the adjugate matrix.

From the particular form of $\gamma(k)$, we deduce that the entries of $g(k)$ will be fractions of finite-degree polynomials of $\sin k_x, \cos k_x, \sin k_y, \cos k_y$. In particular, the numerator and denominator are both of degree ≤ 2 (in general the degree is $\leq 2\chi$, with χ the number of virtual layers).

3.2.3 Parent Hamiltonians

In this section we introduce two types of quadratic Hamiltonians that have a given GFPEPS as ground state. In the first part, we introduce a family of parent Hamiltonians taking advantage of the gaussianity of the state: we will write the matrix of the coefficients of the quadratic operators directly from the correlation matrix of the state. In this family, the Hamiltonians in general will have very different properties from each other depending on the correlation matrix and on the choice of the spectrum. The second type of Hamiltonian corresponds to the parent Hamiltonian constructed in section 2.2.2: taking advantage of the fact that the state is a PEPS and from the condition (2.33), we can search for a parent Hamiltonian that is guaranteed to be local and frustration-free.

Parent Hamiltonians for gaussian states

For pure translational invariant GFPEPS ρ described by the covariant matrix $g^{ab}(k)$, we define a class of quadratic Hamiltonians

$$\hat{H} = \frac{i}{2} \sum_k \sum_{a,b} \varepsilon(k) g^{ab}(k) \hat{d}_k^b \hat{d}_k^{a\dagger}, \quad (3.94)$$

where $\varepsilon(k) \geq 0$. It is not hard to see that ρ is actually a ground state of this Hamiltonian. We notice that the 2×2 case, when we allow only one physical fermion per site ($f = 1$), has already been proved in section 3.2.1. The energy bands in this case are given by $\pm\varepsilon(k)$. Furthermore, all parent Hamiltonians for a two level system must be in this form: this must hold in particular for the second type of Hamiltonian we are going to define in the next section. This fact is not true in general for $f > 1$.

We consider now the general case, with $a, b = 1, \dots, 2f$. If we want to minimize $\text{Tr}(\hat{H}\rho')$ by a translational invariant gaussian state ρ' , we should just minimize for each k independently since, from 3.68, we can write:

$$\text{Tr}(\hat{H}\rho') = \sum_k \text{tr}(h(k)g'(k)), \quad (3.95)$$

where $h(k) = \varepsilon(k)g(k)$ and $g'(k)$ is the covariant matrix of the minimizing state we want to find. Then, since a covariant matrix of a pure state must be antihermitian and unitary, $g(k)$ can be diagonalized in an antihermitian, unitary and diagonal matrix $d(k)$, that therefore has only $\pm i$ diagonal entries: moreover, if $g(k)$ is continuous in k in the thermodynamic limit, the number of $+i$ eigenvalues must remain the same over k ; after a permutation of the diagonal elements, all $d(k)$ matrices are the same for every k , then we can skip the k dependence. The problem now reduces to minimize

$$\text{tr}(g(k)g'(k)) = \text{tr}(U(k)g(k)U(k)^\dagger U(k)g'(k)U(k)^\dagger) =: \text{tr}(d d'(k)) \quad (3.96)$$

over the matrices $d'(k) := U(k)g'(k)U(k)^\dagger$, where $U(k)$ is the unitary transformation that diagonalize $g(k)$ for each k : $U(k)g(k)U(k)^\dagger = d$. Then it is clear that the antihermitian and unitary matrix $d'(k)$ must be exactly equal to d to reach the energy minimum. Then we have $g'(k) = g(k)$ for each k , that means ρ is actually the ground state of the Hamiltonian \hat{H} .

We can now discuss some properties of the system described by this family of Hamiltonians when we make particular choices for $\varepsilon(k)$ [19], remembering that we have

$$h(k) = \varepsilon(k) \left(A + B \frac{\text{Adj}(D + \gamma(k))}{q(k)} B^T \right). \quad (3.97)$$

To make some arguments, in the thermodynamic limit (when $N \rightarrow +\infty$ but the lattice is still discrete), we define the Fourier transform and Fourier antitransform in two dimensions of a function $f(r)$ ($r = (x, y)$, discrete variable) as

$$\begin{aligned} f(k) &= \sum_r e^{-ik \cdot r} f(r), \\ f(r) &= \int \frac{d^2 k}{2\pi} e^{ik \cdot r} f(k). \end{aligned} \quad (3.98)$$

First of all we distinguish the cases in which $q(k) = \det(D + \gamma(k))$ is always $\neq 0$ for every k , from the cases in which it is 0 somewhere.

- When $q(k) \neq 0$ for every k , we discuss two main cases depending on the choice of $\varepsilon(k)$.
 - If we choose $\varepsilon(k) = q(k)$, in the above formula (3.97) we are left with no trigonometric polynomials in the denominator, so $h(k)$ is a trigonometric polynomial of finite degrees itself; this implies that in Fourier antitransform, the matrix $H_{rs} = H(r - s)$ of the coefficients is zero when the distance $|r - s|$ is greater than the degree of the polynomial. To see this, let's consider a generic $f(k)$, finite-degree polynomial of $\sin k_x, \cos k_x, \sin k_y, \cos k_y$, that therefore can be written as

$$f(k) = \sum_{|s| < R} a_s e^{-ik \cdot s}, \quad (3.99)$$

with $s = (x, y) \in \mathbb{Z}^2$, $|s| = x + y$ and R the degree of the polynomial. Then, its antitransform reads

$$f(r) = \sum_{|s| < R} a_s \int \frac{d^2 k}{2\pi} e^{ik \cdot (r-s)} = \sum_{|s| < R} a_s \delta_{rs} = \begin{cases} a_r, & |r| < R \\ 0, & |r| > R \end{cases}. \quad (3.100)$$

Applying an analogous argument for $h(k)$ and $H(r - s)$, we conclude that the Hamiltonian is strictly local. Furthermore, in the two bands case ($f = 1$), since $\varepsilon(k) > 0$, the two bands described by $\pm\varepsilon(k)$ do not touch, so the system is gapped. A gapped Hamiltonian is obtained also in the generic case $f \geq 1$ [19].

- If we choose $\varepsilon(k) = 1$, then $h(k) = g(k)$ that is a fraction of finite-degree trigonometric polynomials. In this case the hopping terms of the Hamiltonian decay exponentially in r : the Hamiltonian is not strictly local, but it is generically said to be short range. This is due to the fact that $h(k)$ is infinitely differentiable and then, from (C.4), $H(r)$ decay faster than any polynomial in $|r|$. In the two bands case, it is clear that the energy bands are flat in momentum space and are separated by a gap $\Delta E = 2$. Even here, a gapped Hamiltonian is obtained also in the generic case $f \geq 1$.
- We consider now the case $q(k) = 0$ for some k . The correlations now decay depending on the differentiability of $g(k)$. In particular, from (C.3) (extended in two dimension [8]), if $g(k)$ has the p th derivative discontinuous, then $G(r)$ decays faster than $|r|^{-2-p}$. This, in particular, implies that every local parent Hamiltonian we can construct must be gapless, since we know that the correlations of the ground state of gapped and local Hamiltonians decay exponentially.
 - If we choose $\varepsilon(k) = 1$ (then $h(k) = g(k)$), as in the case $d(k) \neq 0$, we still obtain a gapped Hamiltonian. However, for what we have just said, this Hamiltonian cannot be local: indeed, the hopping terms decay as the correlations of the GFPEPS, namely algebraically.
 - Instead, if we choose $\varepsilon(k) = q(k)$, the singularity in $h(k)$ cancels and we obtain a local Hamiltonian. However, since $\varepsilon(k) = 0$ for some k (in the two bands case the two bands touch), the Hamiltonian is not gapped.

Construction of the frustration-free and local parent Hamiltonian

Following the same philosophy of the section 2.2.2, we show now how to construct a parent Hamiltonian for a GFPEPS such that is local and frustration-free. We are going to search for local terms of the Hamiltonian that act on the four sites of a cell of the lattice, i.e. on a 2×2 plaquette. We first construct the state ρ_{\square} , analogous to (2.32), on the plaquette by applying the operator (3.16) of the four sites of the cell, applying then the projectors (3.18) and (3.19) only on the four internal bonds and tracing out the virtual modes:

$$\rho_{\square} = \text{Tr}_V(\hat{\Omega}_{\square}\rho_{\Phi}), \quad (3.101)$$

where Ω_{\square} is the product of the four projectors and ρ_{Φ} the density matrix of the fiducial state.

We search for an Hamiltonian \hat{h} in the form $\hat{h} = \hat{A}^{\dagger}\hat{A}$, with \hat{A} an operator constructed by a linear combination of the physical Majorana's operators of the plaquette: $\hat{A} = v_r^a \hat{c}_r^a$, with v_r^a complex coefficients. In this form, the Hamiltonian satisfies the requirements of hermiticity and semi-positivity as we already shown; furthermore, \hat{H} is quadratic, as it must be to guarantee the gaussianity of the ground state. Rewriting $\hat{h} = ih_{rs}^{ab} \hat{c}_s^b \hat{c}_r^a$, the matrix h of the coefficients is $h_{rs}^{ab} = -iv_r^a v_s^{b*}$. We would like to rescale the Hamiltonian adding a term proportional to the identity in order to find an antisymmetric and real matrix of

coefficients h , as in our conventions (3.6). This rescaling does not change the ground state. In particular, we redefine h by

$$h_{rs}^{ab} = \frac{v_r^a v_s^{b*} - v_r^{a*} v_s^b}{2i}, \quad (3.102)$$

or, if we consider v as a complex vector with $8f$ components,

$$h = \frac{vv^\dagger - (vv^\dagger)^T}{2i}. \quad (3.103)$$

One can see that the new \hat{h} becomes

$$\begin{aligned} \hat{h} &= \frac{1}{2} \sum_{rs} \sum_{ab} (v_r^a v_s^{b*} \hat{c}_s^b \hat{c}_r^a - v_r^{a*} v_s^b \hat{c}_s^b \hat{c}_r^a) \\ &= \frac{1}{2} \sum_{rs} \sum_{ab} (2v_r^a v_s^{b*} \hat{c}_s^b \hat{c}_r^a - v_r^{a*} v_s^b \{\hat{c}_s^b, \hat{c}_r^a\}) \\ &= \hat{A}^\dagger \hat{A} - v^\dagger v \mathbb{1}, \end{aligned} \quad (3.104)$$

so the change implies only a rescale of the energy.

To find the vector v we need then to impose the minimization of the energy of the state ρ_\square , that is $\text{Tr}(\hat{h}\rho_\square)$. If we call g the covariant matrix of ρ_\square , the energy can be written in a matrix way:

$$\begin{aligned} \text{Tr}(\hat{h}\rho_\square) &= i \sum_{rs} \sum_{ab} h_{rs}^{ab} \text{Tr}(\hat{c}_s^b \hat{c}_r^a \rho_\square) \\ &= \frac{i}{2} \sum_{rs} \sum_{ab} h_{rs}^{ab} \text{Tr}([\hat{c}_s^b, \hat{c}_r^a] \rho_\square) \\ &= \sum_{rs} \sum_{ab} h_{rs}^{ab} g_{sr}^{ba} \\ &= \text{tr}(hg) \\ &= \text{tr}\left(\frac{vv^\dagger - (vv^\dagger)^T}{2i} g\right) \\ &= -i \text{tr}(vv^\dagger g) \\ &= -iv^\dagger g v. \end{aligned} \quad (3.105)$$

Imposing that v is normalized (since a normalization factor only change the Hamiltonian by a multiplicative factor), the minimum energy is reached when v is an eigenvector of the eigenvalue with minimum imaginary part. We remember that g is a correlation matrix and then its eigenvalues are all pure imaginary in the interval from $-i$ to i . For example, in the case g has a $-i$ eigenvalue, a corresponding eigenvector is a good choice for v : $\Gamma v = -iv$ and then $\text{Tr}(\hat{h}\rho_\square) = -1$. In chapter 5, we will see that our GFPEPS allows the $-i$ eigenvalue for the correlation matrix of the plaquette: furthermore, it will turn out that $-i$ is not degenerate, allowing us to find exactly one parent Hamiltonian with local terms on the 2×2 plaquette.

Once we find the local Hamiltonians \hat{h}_r , we should sum up over all the possible 2×2 plaquettes; for a lattice on a torus they are exactly equal to the number of sites N :

$$\hat{H} = \sum_r \hat{h}_r, \quad (3.106)$$

obtaining a local and frustration free Hamiltonian for the GFPEPS.

Chapter 4

Topology and GFPEPS

4.1 Basic concepts of Topological Condensed Matter

In this section we are going to introduce some concepts of Topological Condensed Matter. In particular, we are interested in the topological property known as *Chern number* that will be computed for the model studied in the following chapter.

4.1.1 Adiabatic theorem

We know that for a time independent hamiltonian \hat{H} , the general solution of the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \quad (4.1)$$

can be found from the solution of the eigenproblem for \hat{H} , that consists in finding an orthonormal basis $\{|\phi_n^\alpha\rangle\}_{n,\alpha}$ such that

$$\hat{H} |\phi_n^\alpha\rangle = E_n |\phi_n^\alpha\rangle, \quad (4.2)$$

for certain real E_n , the possible energies of the system. Here, the index n corresponds to the energy level, while α counts the possible degeneracy of a certain level. The orthogonality condition reads

$$\langle \phi_n^\alpha | \phi_m^\beta \rangle = \delta_{nm} \delta^{\alpha\beta}. \quad (4.3)$$

A generic solution of the Schrödinger equation is then given by

$$|\psi(t)\rangle = \sum_{n,\alpha} c_n^\alpha e^{-\frac{i}{\hbar} E_n t} |\phi_n^\alpha\rangle, \quad (4.4)$$

with generic complex coefficients c_n^α .

Let's consider now a family of Hamiltonians $\hat{H}(\mathbf{R})$ depending continuously on a vector of parameters \mathbf{R} [21][2]. First, we solve the eigenproblem for each \mathbf{R} :

$$\hat{H}(\mathbf{R}) |\phi_n^\alpha(\mathbf{R})\rangle = E_n(\mathbf{R}) |\phi_n^\alpha(\mathbf{R})\rangle, \quad (4.5)$$

where

$$\langle \phi_n^\alpha(\mathbf{R}) | \phi_m^\beta(\mathbf{R}) \rangle = \delta_{nm} \delta^{\alpha\beta} \mathbf{R}. \quad (4.6)$$

We consider now the evolution of the quantum system when we change \mathbf{R} in time, following a curve $\mathbf{R}(t)$ in the parameter space, from t_i to t_f . The new Schrödinger equation reads

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H}(\mathbf{R}(t)) |\psi(t)\rangle. \quad (4.7)$$

The Hamiltonian evolution is then no more time independent. We impose the following form for the solution of the time dependent Schrödinger equation:

$$|\psi(t)\rangle = \sum_{n,\alpha} c_n^\alpha(t) e^{i\theta_n(t)} |\phi_n^\alpha(\mathbf{R}(t))\rangle, \quad (4.8)$$

where $\theta(t)$ is called the *dynamic phase factor* defined by

$$\theta_n(t) = -\frac{1}{\hbar} \int_0^t E_n(\mathbf{R}(\tau)) d\tau. \quad (4.9)$$

Inserting (4.8) in (4.7), after some cancellation due to the convenient definition of $\theta_n(t)$, we find

$$\sum_{n,\alpha} e^{i\theta_n(t)} \left(\frac{d}{dt} (c_n^\alpha(t)) |\phi_n^\alpha(\mathbf{R}(t))\rangle + c_n^\alpha(t) \frac{d}{dt} |\phi_n^\alpha(\mathbf{R}(t))\rangle \right) = 0. \quad (4.10)$$

Applying on the left $\langle \phi_m^\beta(\mathbf{R}(t)) |$ we find an equation for $c_m^\beta(t)$:

$$\begin{aligned} \frac{d}{dt} c_m^\beta(t) &= - \sum_{n\alpha} e^{i(\theta_n(t) - \theta_m(t))} c_n^\alpha(t) \langle \phi_m^\beta(\mathbf{R}(t)) | \frac{d}{dt} |\phi_n^\alpha(\mathbf{R}(t))\rangle \\ &= - \sum_{\alpha} c_m^\alpha(t) \langle \phi_m^\beta(\mathbf{R}(t)) | \frac{d}{dt} |\phi_m^\alpha(\mathbf{R}(t))\rangle \\ &\quad - \sum_{n \neq m, \alpha} e^{i(\theta_n(t) - \theta_m(t))} c_n^\alpha(t) \langle \phi_m^\beta(\mathbf{R}(t)) | \frac{d}{dt} |\phi_n^\alpha(\mathbf{R}(t))\rangle. \end{aligned} \quad (4.11)$$

To find $\langle \phi_m^\beta(\mathbf{R}(t)) | \frac{d}{dt} |\phi_n^\alpha(\mathbf{R}(t))\rangle$ for $m \neq n$, we can take (4.5), derive by t and apply $\langle \phi_m^\beta(\mathbf{R}(t)) |$ on the left, obtaining

$$\langle \phi_m^\beta(\mathbf{R}(t)) | \frac{d}{dt} |\phi_n^\alpha(\mathbf{R}(t))\rangle = \frac{\langle \phi_m^\beta(\mathbf{R}(t)) | \frac{d}{dt} \hat{H}(\mathbf{R}(t)) | \phi_n^\alpha(\mathbf{R}(t)) \rangle}{E_n(\mathbf{R}(t)) - E_m(\mathbf{R}(t))}. \quad (4.12)$$

This equation holds only if different energy levels remain separated by gaps $\forall t$ in the interval $[t_i, t_f]$.

We notice that such a term is negligible if the change of R and then of \hat{H} is small compared with the energy gap between two energy levels

$$\frac{\| \frac{d}{dt} \mathbf{R} \|}{\| \mathbf{R} \|} \ll \frac{\Delta E}{\hbar}; \quad (4.13)$$

the approximation can be done since the presence of oscillation term $e^{i(\theta_n(t)-\theta_m(t))}$ in (4.11) that, after the integration over dt , keeps the contribution small. We call this process *adiabatic* since we slowly change the parameters during the evolution of the system. The resulting equation for $c_m^\beta(t)$ becomes

$$\frac{d}{dt}c_m^\beta(t) = -\sum_{\alpha} c_m^\alpha(t)\langle\phi_m^\beta(\mathbf{R}(t))|\frac{d}{dt}|\phi_m^\alpha(\mathbf{R}(t))\rangle. \quad (4.14)$$

Defining

$$X_m^{\beta\alpha}(t) := -\langle\phi_m^\beta(\mathbf{R}(t))|\frac{d}{dt}|\phi_m^\alpha(\mathbf{R}(t))\rangle, \quad (4.15)$$

in the matrix form, the equation becomes

$$\frac{d}{dt}c_n(t) = X_n(t)c_n(t), \quad (4.16)$$

where we remember that m is the index of the energy level and the dimensions of X_n is given by the degeneracy of the level. Furthermore, we notice that $X(t)$ is antihermitian: this can be shown from the orthonormality conditions (4.6), taking the time derivative. If we call $U_n(t)$ the matrix that solve the equation

$$\frac{d}{dt}U_n(t) = X_n(t)U_n(t) \quad (4.17)$$

with initial condition

$$U_n(0) = \mathbb{1} \quad (4.18)$$

for each n , then the solution of (4.16) is

$$c_n(t) = U_n(t)c_n(0). \quad (4.19)$$

Furthermore, since $X(t)$ is antihermitian, $U(t)$ is unitary¹.

The solution of the Schrödinger equation (4.8) is then

$$\begin{aligned} |\psi(t)\rangle &= \sum_{n,\alpha,\beta} U_n^{\alpha\beta}(t)c_n^\beta(0)e^{i\theta_n(t)}|\phi_n^\alpha(\mathbf{R}(t))\rangle \\ &= \sum_{n,\alpha,\beta} U_n^{\alpha\beta}(t)\langle\phi_n^\beta(0)|\psi(0)\rangle e^{i\theta_n(t)}|\phi_n^\alpha(\mathbf{R}(t))\rangle. \end{aligned} \quad (4.20)$$

In particular, we notice that if the initial state is in the eigenspace of $E_n(\mathbf{R}(0))$, then the adiabatic process keeps the state in the corresponding eigenspace, the one of $E_n(\mathbf{R}(t))$. We specify now this result for a non-degenerate energy E_n : for that level, the unitary

¹Indeed, if we take the hermitian conjugate of (4.17), we get: $\frac{d}{dt}U_n(t)^\dagger = U_n(t)^\dagger X_n(t)^\dagger = -U_n(t)^\dagger X_n(t)$ due the anti-hermiticity of $X_n(t)$. Then, $\frac{d}{dt}(U_n(t)^\dagger U_n(t)) = \frac{d}{dt}U_n(t)^\dagger U_n(t) + U_n(t)^\dagger \frac{d}{dt}U_n(t) = -U_n(t)^\dagger X_n(t)U_n(t) + U_n(t)^\dagger X_n(t)U_n(t) = 0$. Then $U_n(t)^\dagger U_n(t)$ is constant in time and, since at $t = 0$ it is equal to $\mathbb{1}$ for (4.18), $U_n(t)$ is unitary.

matrix $U_n(t)$ becomes simply a phase, that we indicate with $U_n(t) = e^{i\gamma_n(t)}$. $\gamma_n(t)$ is called *geometric phase* and it is given from (4.17) and (4.15):

$$\begin{aligned}\gamma_n(t) &= i \int_{t_i}^t \langle \phi_n(\mathbf{R}(\tau)) | \frac{d}{d\tau} | \phi_n(\mathbf{R}(\tau)) \rangle d\tau \\ &= i \int_{t_i}^t \langle \phi_n(\mathbf{R}) | \nabla_{\mathbf{R}} | \phi_n(\mathbf{R}) \rangle(\tau) \cdot \frac{d\mathbf{R}(\tau)}{d\tau} d\tau \\ &= i \int_{\mathcal{C}} \langle \phi_n(\mathbf{R}) | \nabla_{\mathbf{R}} | \phi_n(\mathbf{R}) \rangle \cdot d\mathbf{R},\end{aligned}\tag{4.21}$$

where the last integral is done along the curve \mathcal{C} in the parameters space, independently from the choice of the time-dependence, i.e. its parametrization. Then, if we start from the eigenstate $|\phi_n(\mathbf{R}(0))\rangle$ of $E_n(\mathbf{R}(0))$, the state at time t after the adiabatic process will be

$$|\psi(t)\rangle = e^{i\gamma_n(t)} e^{i\theta_n(t)} |\phi_n(\mathbf{R}(t))\rangle,\tag{4.22}$$

that means that the state gains a phase beyond the dynamic phase θ_n .

4.1.2 Berry phase

The non-dynamical phase $\gamma_n(t)$ appearing in the adiabatic solution of the time-dependent Schrödinger equation has interesting properties and physical applications. First, as we just noted, $\gamma_n(t)$ is geometric, meaning that it depends only on the path from $\mathbf{R}(0)$ to $\mathbf{R}(t)$, but not on the time-dependence of travel along this path (provided that, if we want to find the state $|\psi(t)\rangle$ by (4.22), the adiabatic approximation must hold and so the travel must be slow enough). From now on, we will write the Berry phase in function of the curve in the parameters space. It is useful to define the *Berry connection* $\mathbf{A}_n(\mathbf{R})$ on the parameter space:

$$\mathbf{A}_n(\mathbf{R}) := i \langle \phi_n(\mathbf{R}) | \nabla_{\mathbf{R}} | \phi_n(\mathbf{R}) \rangle.\tag{4.23}$$

The Berry phase can then be written simply as

$$\gamma_n(\mathcal{C}) = \int_{\mathcal{C}} \mathbf{A}_n(\mathbf{R}) \cdot d\mathbf{R}.\tag{4.24}$$

We remember that $|\phi_n(\mathbf{R})\rangle$ is the eigenstate of the non degenerate level n of the Hamiltonian $H(\mathbf{R})$: for each \mathbf{R} , its definition is independent from a choice of a phase. Let's suppose we redefine the eigenstate by

$$|\phi_n(\mathbf{R})\rangle \rightarrow e^{i\alpha(\mathbf{R})} |\phi_n(\mathbf{R})\rangle,\tag{4.25}$$

with $\alpha(\mathbf{R})$ a smooth function of \mathbf{R} . Both the connection and the Berry phase are *gauge dependent*, meaning that they transform under the above transformation in the following way:

$$\begin{aligned}\mathbf{A}_n(\mathbf{R}) &\rightarrow \mathbf{A}_n(\mathbf{R}) - \nabla_{\mathbf{R}}\alpha(\mathbf{R}), \\ \gamma_n(\mathcal{C}) &\rightarrow \gamma_n(\mathcal{C}) - \alpha(\mathbf{R}(t)) + \alpha(\mathbf{R}(0)).\end{aligned}\tag{4.26}$$

We notice that for a generic open path the geometric phase can be cancelled out by a suitable choice of a gauge transformation $\alpha(\mathbf{R})$. However, as noted Berry [3], this cancellation cannot be done in the case of a close path, from $\mathbf{R}(0)$ to $\mathbf{R}(t) = \mathbf{R}(0)$. In this case the geometric phase is gauge independent and it is called *Berry phase*:

$$\gamma_n(\mathcal{C}) = \oint_{\mathcal{C}} \mathbf{A}_n(\mathbf{R}) \cdot d\mathbf{R}, \quad (4.27)$$

where \mathcal{C} is now a circuit. To express the integral in a explicitly gauge invariant way, we introduce the *Berry curvature* $F_{\mu\nu}(\mathbf{R})$ by

$$F_{n\mu\nu}(\mathbf{R}) := \frac{\partial}{\partial R^\mu} A_{n\nu}(\mathbf{R}) - \frac{\partial}{\partial R^\nu} A_{n\mu}(\mathbf{R}), \quad (4.28)$$

where R^μ and A_μ are the components of the vectors \mathbf{R} and \mathbf{A} respectively. In terms of differential forms, if $A_n u$ are the components of a 1-form, $F_{\mu\nu}$ are the components of a 2-form that is the differential of the previous one. Then, by the Stoke's theorem, if the space is simply connected, we have

$$\gamma_n(\mathcal{C}) = \oint_{\mathcal{C}} A_{n\mu}(\mathbf{R}) dR^\mu = \int_{\mathcal{S}(\mathcal{C})} \frac{1}{2} F_{n\mu\nu}(\mathbf{R}) dR^\mu \wedge dR^\nu, \quad (4.29)$$

where $\mathcal{S}(\mathcal{C})$ is a generic surface with the circuit \mathcal{C} as a boundary.

We conclude with a result coming from algebraic topology: the integral of the Berry curvature on a closed 2-dimensional manifold is always a multiple of 2π [9]; this leads to the definition of the *Chern number* C_n of the energy level n

$$C_n = \frac{1}{4\pi} \int_{\mathcal{S}} F_{n\mu\nu}(\mathbf{R}) dR^\mu \wedge dR^\nu, \quad (4.30)$$

which has to be an integer. Physically, there is a reason why the Chern number should be an integer. Let's consider a simply connected circuit that divides the above surface \mathcal{S} in two surfaces with border: $\mathcal{S}_1(\mathcal{C})$ and $\mathcal{S}_2(\mathcal{C})$ (we should change the sign of one contribution if we want to keep the same orientation for \mathcal{C}).

$$C_n = \frac{1}{2\pi} \left(\frac{1}{2} \int_{\mathcal{S}_1(\mathcal{C})} F_{n\mu\nu}(\mathbf{R}) dR^\mu \wedge dR^\nu - \frac{1}{2} \int_{\mathcal{S}_2(\mathcal{C})} F_{n\mu\nu}(\mathbf{R}) dR^\mu \wedge dR^\nu \right). \quad (4.31)$$

The two contribution corresponds exactly to the Berry phase: however, since this phase is defined modulo 2π , we could obtain two results that can be different only for $2\pi m$, with m integer:

$$C_n = \frac{1}{2}(2\pi m) = m \in \mathbb{Z}. \quad (4.32)$$

It can also be proved [1] that the sum of the Chern numbers for all energy levels (here we consider no degeneracy for each level) is equal to zero:

$$\sum_n C_n = 0. \quad (4.33)$$

4.1.3 Berry phase in Bloch bands

In the previous two sections we introduced the Berry phase considering the adiabatic evolution of a system under a slow change of a set of parameters (\mathbf{R}) of the Hamiltonian. Now, instead, we will apply the same mathematical structure to crystalline solids.

Within the independent electron approximation, the band structure of a crystal is determined by the single electron Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\mathbf{r}), \quad (4.34)$$

where $V(\mathbf{r}) = V(\mathbf{r} + \mathbf{a})$ is a periodic potential and \mathbf{a} a vector of the Bravais lattice. In a crystal, each eigenstate of the Hamiltonian H is also eigenstate of the translation operators $T_{\mathbf{a}}$, for each \mathbf{a} in the lattice. In particular, due to Bloch's theorem, each eigenstate can be written as

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{r}\cdot\mathbf{k}} u_{n\mathbf{k}}(\mathbf{r}), \quad (4.35)$$

where n is the index of the energy state, $u_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r} + \mathbf{a})$ is a cell-periodic function and $\hbar\mathbf{k}$ is the crystal momentum that resides in the Brillouin zone. The eigenproblem for the Hamiltonian (4.34) reads

$$\hat{H}\psi_{n\mathbf{k}}(\mathbf{r}) = E_{n\mathbf{k}}\psi_{n\mathbf{k}}(\mathbf{r}). \quad (4.36)$$

From equation (4.35) and from the momentum operator definition $\hat{p} = -i\hbar\nabla$, we get

$$\left(\frac{(\hbar\mathbf{k} - i\hbar\nabla)^2}{2m} + V(\mathbf{r}) \right) u_{n\mathbf{k}}(\mathbf{r}) = E_{n\mathbf{k}}u_{n\mathbf{k}}(\mathbf{r}). \quad (4.37)$$

If we define the *Bloch Hamiltonian* as

$$\hat{H}(\mathbf{k}) := e^{-i\mathbf{r}\cdot\mathbf{k}} \hat{H} e^{i\mathbf{r}\cdot\mathbf{k}} = \left(\frac{(\hbar\mathbf{k} - i\hbar\nabla)^2}{2m} + V(\mathbf{r}) \right), \quad (4.38)$$

we notice that we recover the same mathematical framework of the adiabatic evolution: we have an Hamiltonian \mathbf{k} -dependent, instead of $\hat{H}(\mathbf{R})$, with eigenstates $|u_{n\mathbf{k}}\rangle =: |u_n(\mathbf{k})\rangle$, instead of the previous $|\phi_n(\mathbf{R})\rangle$ (again, we restrict ourself to the non-degenerate case that leads to an abelian gauge connection). So, for example, if \mathbf{k} is forced to vary in momentum space along a circuit, the state will pick up a Berry phase

$$\gamma_n(t) = i \oint_{\mathcal{C}} \langle u_n(\mathbf{k}) | \nabla_{\mathbf{k}} | u_n(\mathbf{k}) \rangle \cdot d\mathbf{k}. \quad (4.39)$$

In the last part of this section we restrict ourself to the cases of three and two dimensional space and we give an explicit computation of the Chern number in a two band system. In three dimensional space, the momentum \mathbf{k} is a three vector $\mathbf{k} = (k^1, k^2, k^3)$. From the Berry curvature we can construct a three dimensional vector $\mathbf{F}_n(\mathbf{k})$, defining its components by $F_n^i(\mathbf{k}) := \epsilon^{ijk} F_{njk}(\mathbf{k})$, where $F_{njk}(\mathbf{k})$ is given by (4.28), with the role of \mathbf{R} played here by \mathbf{k} . Then we can write equivalently

$$\mathbf{F}_n(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathbf{A}_n(\mathbf{k}). \quad (4.40)$$

The Berry phase along a circuit \mathcal{C} in the momentum space becomes

$$\gamma_n(\mathcal{C}) = \int_{S(\mathcal{C})} \mathbf{F}_n(\mathbf{k}) \cdot d\mathbf{S}. \quad (4.41)$$

We notice the analogy of \mathbf{A}_n with the vector potential of electromagnetism and \mathbf{F}_n with the magnetic field. In two dimensions the situation is even simpler: $\mathbf{k} = (k^1, k^2)$, $\mathbf{A}_n(\mathbf{k})$ is a two vector and $F_{nij}(\mathbf{k})$ has only one independent component, say

$$F_{n12}(\mathbf{k}) = \frac{\partial}{\partial k^1} A_{n2}(\mathbf{k}) - \frac{\partial}{\partial k^2} A_{n1}(\mathbf{k}) =: 2F_n(\mathbf{k}). \quad (4.42)$$

The Berry phase, given by the integral (4.29), is then simply the volume integral

$$\gamma_n(\mathcal{C}) = \int_{S(\mathcal{C})} F_n(\mathbf{k}) dk^1 dk^2 \quad (4.43)$$

over a surface enclosed by the circuit, while the Chern number becomes

$$C_n = \frac{1}{2\pi} \int_{\text{BZ}} F_n(\mathbf{k}) dk^1 dk^2 \quad (4.44)$$

where the integral is done over the Brillouin zone $\text{BZ} = [0, 2\pi] \times [0, 2\pi]$.

We give now the explicit formula of the Chern number for a two level system described by the Bloch Hamiltonian

$$\hat{H}(\mathbf{k}) = \boldsymbol{\sigma} \cdot \mathbf{h}(\mathbf{k}) = \begin{pmatrix} h_z(\mathbf{k}) & h_x(\mathbf{k}) - ih_y(\mathbf{k}) \\ h_x(\mathbf{k}) + ih_y(\mathbf{k}) & -h_z(\mathbf{k}) \end{pmatrix}, \quad (4.45)$$

where $\boldsymbol{\sigma}$ is the vector of the Pauli matrices and $\mathbf{h}(\mathbf{k})$ a three-vector. We rewrite the Hamiltonian above in terms of $h(\mathbf{k}), \theta(\mathbf{k}), \phi(\mathbf{k})$, the spherical components of $\mathbf{h}(\mathbf{k})$:

$$\begin{pmatrix} h_x(\mathbf{k}) \\ h_y(\mathbf{k}) \\ h_z(\mathbf{k}) \end{pmatrix} =: \begin{pmatrix} h(\mathbf{k}) \sin \theta(\mathbf{k}) \cos \phi(\mathbf{k}) \\ h(\mathbf{k}) \sin \theta(\mathbf{k}) \sin \phi(\mathbf{k}) \\ h(\mathbf{k}) \cos \theta(\mathbf{k}) \end{pmatrix}. \quad (4.46)$$

The Hamiltonian becomes

$$\hat{H}(\mathbf{k}) = h(\mathbf{k}) \begin{pmatrix} \cos \theta(\mathbf{k}) & \sin \theta(\mathbf{k}) e^{-i\phi(\mathbf{k})} \\ \sin \theta(\mathbf{k}) e^{i\phi(\mathbf{k})} & -\cos \theta(\mathbf{k}) \end{pmatrix}. \quad (4.47)$$

The energy band structure is easily computable and is given by

$$E_{\pm}(\mathbf{k}) = \pm h(\mathbf{k}). \quad (4.48)$$

We notice that the system is gapped if and only if $h(\mathbf{k}) > 0 \forall \mathbf{k}$. After computing the eigenvectors, one can calculate the Chern number of the lowest energy band and find

$$C_- = \frac{1}{4\pi} \int_{\text{BZ}} \mathbf{h}'(\mathbf{k}) \cdot \left(\frac{\partial \mathbf{h}'(\mathbf{k})}{\partial k^1} \times \frac{\partial \mathbf{h}'(\mathbf{k})}{\partial k^2} \right) dk^1 dk^2, \quad (4.49)$$

where $\mathbf{h}'(\mathbf{k})$ is the normalized vector $\frac{\mathbf{h}(\mathbf{k})}{h(\mathbf{k})}$.

The above formula for Chern number is still valid for two-bands systems describing fermions, i.e. systems with Hamiltonians in the form

$$\hat{H} = \sum_{\mathbf{k}} \hat{d}_k^{a\dagger} (\sigma \cdot \mathbf{h}(\mathbf{k}))_{ab} \hat{d}_k^b, \quad (4.50)$$

where \hat{d}_k^a are the operators defined in (3.40).

The Chern number is a relevant property of systems called *topological insulators*, where the Chern number of the occupied bands, defined as the sum of the Chern numbers of these bands, is different from zero. A topological insulator, like an ordinary insulator, has a bulk energy gap separating the highest occupied electronic band from the lowest empty band. The surface, however, necessarily has gapless electronic states because it stands in the phase transition region between the insulator and the vacuum, that trivially has Chern number 0. These electronic states are also called *chiral edge states* and are protected against local perturbations of the bulk. For our purpose, a chiral GFPEPS is simply a GFPEPS with non trivial Chern number: however, the right definition would involve these chiral edge states that appears in presence of a boundary.

4.2 Injective GFPEPS and chirality

In this section we show that GFPEPS are related to topology in a particular way. We remember first the concept of injectivity introduced at the end of section 2.2.2 for MPS: an MPS is injective if the map ϕ_r (2.16) from virtual to physical is injective. As we noted, ϕ_r is a map in the valence bond approach: in the fiducial state construction, instead, the corresponding object is the fiducial state $|\phi_r\rangle$ placed on each site of the lattice. The aim of this section is to show that GFPEPS that have an analogous injectivity property (that we are going to define) cannot have a Chern number $C \neq 0$ [19]. For MPS, this property implies that its local parent Hamiltonians are gapped; also for PEPS there are strong reasons to believe that, even if not proved. So, this result is a strong indication that we cannot have a chiral GFPEPS that is a ground state of a gapped local Hamiltonian.

We now define properly injectivity for GFPEPS [19]: starting from the vacuum of the physical+virtual system, consider the procedure of blocking $L_x \times L_y$ sites by tracing over the internal virtual modes; for each block we are left with $d_p = 2fL_xL_y$ physical modes and $d_v = 2\chi(L_x + L_y)$ virtual ones. We then find some matrices A_{\square} ($d_p \times d_p$), B_{\square} ($d_p \times d_v$) and D_{\square} ($d_v \times d_v$) such that they give the GFPEPS described by the correlation matrix G by the usual formula in Fourier transform: $g_{\square}(k) = A_{\square} + B_{\square} (D_{\square} + \gamma_{\square}(k))^{-1} B_{\square}^T$, where now $\gamma_{\square}(k)$ is the correlation matrix of the virtual projector needed to connect the remaining bonds of the lattice, namely the virtual bonds between the various blocks. We say that a GFPEPS is *injective* if there exists a finite blocking size such that $d_p > d_v$ and $\text{rk}(B_{\square}) = d_v$, namely that, in the valence bond perspective, $\gamma_{\square}(k)$ is fully mapped onto the physical space.

To proceed with the proof, given an injective GFPEPS with a certain blocking as above, we use the singular value decomposition (A.1) on B_{\square} : $B_{\square} = V\Sigma U^{\dagger}$ where Σ is a diagonal matrix $d_p \times d_v$, strictly positive since B_{\square} is full rank; here U is an unitary matrix $d_p \times d_p$

and V is $d_p \times d_v$ with orthonormal columns ($V^\dagger V = \mathbb{1}$). Rewriting the decomposition, we obtain

$$g_\square(k) - A = V\Sigma U^\dagger (D_\square + \gamma_\square(k))^{-1} U\Sigma V^\dagger. \quad (4.51)$$

If we apply V^\dagger on the left, V on the right and take the determinant, we get

$$\det(V^\dagger(g_\square(k) - A)V) = \frac{\det \Sigma^2}{\det(D_\square + \gamma_\square(k))}. \quad (4.52)$$

We define now a family of gaussian states with correlation matrices $g^\phi(k)$ with $\phi \in [0, \frac{\pi}{2}]$ given by

$$g_\square^\phi(k) := A_\square + B_\square(D_\square + \gamma_\square^\phi(k))^{-1} B_\square^T, \quad (4.53)$$

where $\gamma_\square^\phi(k)$ is given by the same procedure we can find $\gamma_\square(k)$ except that the starting correlation matrix of the virtual projector is not given by Γ in (3.77), but by Γ^ϕ whose corresponding Γ_h^ϕ and Γ_v^ϕ are given by

$$\Gamma_h^\phi = \Gamma_v^\phi = \begin{pmatrix} 0 & \sin \phi & & & & & & & -\cos \phi \\ -\sin \phi & 0 & \cos \phi & & & & & & \\ & -\cos \phi & 0 & \sin \phi & & & & & \\ & & -\sin \phi & 0 & \cos \phi & & & & \\ & & & -\cos \phi & \ddots & \ddots & & & \\ & & & & \ddots & 0 & \sin \phi & & \\ \cos \phi & & & & & -\sin \phi & 0 & & \end{pmatrix}. \quad (4.54)$$

We remember that the entries of Γ_h^ϕ correspond to the ordering

$$\hat{\gamma}_{1,1}^l, \hat{\gamma}_{1,1}^r, \hat{\gamma}_{1,2}^l, \hat{\gamma}_{1,2}^r, \dots, \hat{\gamma}_{1,N_y}^l, \hat{\gamma}_{1,N_y}^r, \quad (4.55)$$

and for Γ_v^ϕ

$$\hat{\gamma}_{1,1}^u, \hat{\gamma}_{1,1}^d, \hat{\gamma}_{2,1}^u, \hat{\gamma}_{2,1}^d, \dots, \hat{\gamma}_{N_y,1}^u, \hat{\gamma}_{N_y,1}^d. \quad (4.56)$$

We notice that $g_\square(k)$ is recovered for $\phi = 0$: $\cos \phi = 1$ and $\sin \phi = 0$, then the virtual correlations are totally shared by Majorana operators of different sites. Instead, in the case $\phi = \frac{\pi}{2}$, the correlations are all inside each site. The state of $g_\square^{\frac{\pi}{2}}(k)$ is totally disentangled: it is a product state of states living in each site and therefore it is then topologically trivial. Now we just need to show that we can follow the disentangling path connecting $g_\square(k)$ to $g_\square^{\frac{\pi}{2}}(k)$ by an adiabatic process. To do this we notice some properties of (4.52) that, extended for every ϕ , reads:

$$\det(V^\dagger(g_\square^\phi(k) - A)V) = \frac{\det \Sigma^2}{\det(D_\square + \gamma_\square^\phi(k))}. \quad (4.57)$$

We see that the left part is bounded by a constant $M \forall \phi$ since all the matrices involved live in bounded spaces. Furthermore, the numerator of the right part is strictly positive.

This implies that the absolute value of determinant at denominator is strictly greater than 0 $\forall \phi$:

$$q_{\square}^{\phi}(k) := |\det(D_{\square} + \gamma_{\square}^{\phi}(k))| = \frac{\det \Sigma^2}{|\det(V^{\dagger}(g_{\square}^{\phi}(k) - A)V)|} \geq \delta > 0. \quad (4.58)$$

For each ϕ , now we construct a parent Hamiltonian \hat{H}^{ϕ} as defined in (3.94) that has the gaussian state given by $g^{\phi}(k)$ as ground state and with $\varepsilon(k) = q_{\square}(k)$: as we already stated in 3.2.3, these Hamiltonians are local and gapped. We then have constructed a gapped path between our injective GFPEPS and a trivial gaussian state: the two states are then topological equivalent, meaning that the topological property are the same. An injective GFPEPS is then always trivial.

From what we said in the last part of section 2.3.1, injectivity is a strong indication that the local parent Hamiltonians we can construct are gapped: this is true for MPS, but not demonstrated for PEPS. This means that it is highly possible that a GFPEPS with local and gapped Hamiltonian is always topologically trivial.

Chapter 5

Example of chiral GFPEPS and perturbation

The model we are going to study [20] is a chiral GFPEPS with one physical mode per site ($f = 1$) and one virtual layer ($\chi = 1$). We are not going to show why the state is chiral, i.e. why it has a chiral current at the boundary, since we are considering a lattice with periodic boundary conditions and then we cannot visualize any edge. In this contest it is sufficient to know that our state has a non-trivial Chern number: this fact implies, indeed, that if the system is placed on a lattice with boundary immerse in the vacuum, we overcome a point of phase transition going from the system to the vacuum, since the two regions has different Chern numbers. A phase transition at the boundary means that here the system is gapless, allowing the conduction of current. For this state we can construct two types of two-bands parent Hamiltonians. One Hamiltonian is flat-band and gapped, but non-local: in particular, the hopping terms decay as $\frac{1}{r^3}$, and this is compatible with the fact that, in the thermodynamic limit, the correlations of the GFPEPS decay algebraically and not exponentially. Considered as ground state of this Hamiltonian, we can compute the Chern number of the ground state, that happens to be -1 . The other parent Hamiltonian is local and frustration-free: since in the thermodynamic limit it cannot be gapped, otherwise the correlations of the GFPEPS would decay exponentially, it is gapless. In this case, the GFPEPS can be interpreted as being in the quantum phase transition between different phases having different Chern numbers. Under this Hamiltonian, the Chern number defined in (4.44) is not a proper quantity: the Chern number is indeed defined for a totally occupied band well separated in energy from an other bands. Actually, the only Chern number that would make sense is the one calculated from both the touching bands: but then C must be zero for (4.33). From this gapless and local Hamiltonian we will add local quadratic perturbations to enter different gapped topological phases and find the new gaussian ground states.

5.1 Correlation matrix of the GFPEPS

Our GFPEPS is defined from the correlation matrices (3.73), that we choose to be (the order of the Majorana's operator is: $\hat{c}^1, \hat{c}^2, \hat{\gamma}^l, \hat{\gamma}^r, \hat{\gamma}^u, \hat{\gamma}^d$)

$$\begin{aligned} A &= \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \\ B &= \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & -1 \\ -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & -1 & 0 \end{pmatrix} \\ D &= \begin{pmatrix} 0 & 1 - \frac{1}{\sqrt{2}} & -\frac{1}{2} & -\frac{1}{2} \\ -1 + \frac{1}{\sqrt{2}} & 0 & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & 0 & 1 - \frac{1}{\sqrt{2}} \\ \frac{1}{2} & \frac{1}{2} & -1 + \frac{1}{\sqrt{2}} & 0 \end{pmatrix} \end{aligned} \quad (5.1)$$

In D we present a family of GFPEPS in function of λ with the same properties of the one under study, that corresponds to $\lambda = \frac{1}{2}$.

Equivalently, the above correlation matrices correspond to the following operator that generates the fiducial state:

$$\hat{\phi}_r^\dagger = \frac{1}{\sqrt{2}} \mathbb{1} + \frac{1}{2} e^{-i\frac{\pi}{4}} \hat{a}_r^\dagger \hat{h}_r^\dagger + \frac{1}{2} \hat{a}_r^\dagger \hat{v}_r^\dagger. \quad (5.2)$$

To compute the correlation matrix of the GFPEPS, we apply the formula (3.90), from which one we can find the three real components $g^i(k)$ of the correlation matrix in the Fourier space

$$g(k) = \begin{pmatrix} ig^3(k) & g^2(k) + ig^1(k) \\ -g^2(k) + ig^1(k) & -ig^3(k) \end{pmatrix} = ig^i(k) \sigma_i, \quad (5.3)$$

The zero-th component $g^0(k)$ happen to be 0. Defining the determinant $q(k) := \det(D + \gamma(k))$, $g^i(k)$ turns out to be

$$\begin{aligned} g^1(k_x, k_y) &= -\frac{2}{q(k_x, k_y)} \sin^2 \frac{k_x}{2} \sin k_y, \\ g^2(k_x, k_y) &= \frac{1}{2q(k_x, k_y)} (1 - 2(\cos k_x + \cos k_y) + 3 \cos k_x \cos k_y), \\ g^3(k_x, k_y) &= \frac{2}{q(k_x, k_y)} \sin k_x \sin^2 \frac{k_y}{2}, \end{aligned} \quad (5.4)$$

where

$$q(k_x, k_y) = \frac{1}{2} (3 - 2(\cos k_x + \cos k_y) + \cos k_x \cos k_y).$$

It is straightforward to check the properties (3.55) of the correlation matrix $g(k)$. We notice that $q(k_x, k_y)$ is singular in $(0, 0)$, meaning that we cannot actually invert $(D + \gamma(0, 0))$. Nevertheless, going in the thermodynamic limit, k_x and k_y become continuous variables

and we can take the limit at $(0, 0)$ that happens to be well defined. Indeed, for $\|k\| \rightarrow 0$ we can find the following expansions:

$$\begin{aligned}
q(k_x, k_y) &= \frac{1}{4}(k_x^2 + k_y^2) + \mathcal{O}(\|k\|^4), \\
g^1(k_x, k_y) &= -\frac{2k_x^2 k_y}{k_x^2 + k_y^2} + \mathcal{O}(\|k\|^3) \simeq 0, \\
g^2(k_x, k_y) &= -1 + \frac{\frac{3}{2}k_x^2 k_y^2 - \frac{1}{12}(k_x^4 + k_y^4)}{k_x^2 + k_y^2} + \mathcal{O}(\|k\|^4) \simeq -1, \\
g^3(k_x, k_y) &= \frac{2k_x k_y^2}{k_x^2 + k_y^2} + \mathcal{O}(\|k\|^3) \simeq 0.
\end{aligned} \tag{5.5}$$

We would like to get some informations about the decay of correlations. Following the discussion in section 3.2.3, we are in the case $q(k_x, k_y) = 0$ for some (k_x, k_y) : then, the correlations cannot decay faster than $|r|^{-2-d}$, where d is the maximum degree of continuous derivative that we can take. Computing explicitly the derivative for the above $g^i(k_x, k_y)$, it can be found that the first derivatives of $g^1(k_x, k_y)$ and $g^3(k_x, k_y)$ are discontinuous. Then, the entries of the correlation matrix G_{rs} decay slower than $\frac{1}{|r-s|^3}$. We can already say that every local parent Hamiltonian we can construct from this GFPEPS will be surely gapless.

5.2 Parent Hamiltonians

The first Hamiltonian we construct is explicitly given by equation (3.94) with $\varepsilon(k) = 1$. In terms of Majorana's operator, then reads

$$\hat{H} = \frac{i}{2} \sum_{rs} \sum_{a,b}^2 G_{rs}^{ab} \hat{c}_s^b \hat{c}_r^a, \tag{5.6}$$

with G the correlation matrix of our GFPEPS. This Hamiltonian is flat band, with energy gap $\Delta E = 2$ between the two energy bands. Without further arguments, we must conclude that it is not local, otherwise the correlations should decay exponentially.

The second Hamiltonian we construct is given by the standard procedure we explained in the second part of section 3.2.3. The correlation matrix g 8×8 of the physical state ρ_{\square} on the 2×2 plaquette was found to be (the ordering of the Majorana's operator is: $\hat{c}_{1,1}^1, \hat{c}_{1,1}^2, \hat{c}_{1,2}^1, \hat{c}_{1,2}^2, \hat{c}_{2,1}^1, \hat{c}_{2,1}^2, \hat{c}_{2,2}^1, \hat{c}_{2,2}^2$)

$$g = \frac{1}{65} \begin{pmatrix} 0 & -1 & 20 & -16 & -2 & -34 & -8 & 16 \\ 1 & 0 & 16 & -16 & -2 & -2 & 0 & 8 \\ -20 & -16 & 0 & -1 & 8 & 16 & 2 & -34 \\ 16 & 16 & 1 & 0 & 0 & -8 & -2 & 2 \\ 2 & 2 & -8 & 0 & 0 & -1 & 16 & -16 \\ 34 & 2 & -16 & 8 & 1 & 0 & 16 & -20 \\ 8 & 0 & -2 & 2 & -16 & -16 & 0 & -1 \\ -16 & -8 & 34 & -2 & 16 & 20 & 1 & 0 \end{pmatrix}. \tag{5.7}$$

This state is not pure since $g^T g \neq \mathbb{1}$, but still satisfies $g^T g \leq \mathbb{1}$.

The eigenvalue of the above matrix with minimum imaginary part is $-i$ with multiplicity one. Following the procedure in section 3.2.3, we use the corresponding eigenvector v to construct the local terms of the Hamiltonian. With the right normalization, we find

$$v = \frac{1}{2\sqrt{30}} \begin{pmatrix} 5i \\ 1 + 2i \\ 3 - 4i \\ -2 + i \\ -1 - 2i \\ -4 - 3i \\ -2 + i \\ 5 \end{pmatrix}, \quad (5.8)$$

then the physical operator \hat{A} on the plaquettes reads

$$\begin{aligned} \hat{A} = & 5i\hat{c}_{1,1}^1 + (1 + 2i)\hat{c}_{1,1}^2 + (3 - 4i)\hat{c}_{1,2}^1 + (-2 + i)\hat{c}_{1,2}^2 \\ & + (-1 - 2i)\hat{c}_{2,1}^1 + (-4 - 3i)\hat{c}_{2,1}^2 + (-2 + i)\hat{c}_{2,2}^1 + 5\hat{c}_{2,2}^2. \end{aligned} \quad (5.9)$$

We skip know the intermediate passage to find the total parent Hamiltonian. We remember only that first we should find the form of the local Hamiltonian terms \hat{h}_r (in the convention that the matrix of coefficients is antisymmetric). Then we should sum all the local terms over the torus to find the total Hamiltonian $\hat{H} = \sum_r \hat{h}_r$. We give the result in terms of the real components of the matrices of coefficients of \hat{H} in Fourier transform, defined in (3.64) (we avoid writing the zero-th component that happen to be always zero).

$$\begin{aligned} h^1(k_x, k_y) &= -\frac{2}{3} \sin^2 \frac{k_x}{2} \sin k_y, \\ h^2(k_x, k_y) &= \frac{1}{6} (1 - 2(\cos k_x + \cos k_y) + 3 \cos k_x \cos k_y), \\ h^3(k_x, k_y) &= \frac{2}{3} \sin k_x \sin^2 \frac{k_y}{2}. \end{aligned} \quad (5.10)$$

We notice a property that may appear disturbing at first sight, namely

$$h^i(k_x, k_y) = \frac{1}{3} g^i(k_x, k_y) q(k_x, k_y). \quad (5.11)$$

Actually we could be able to anticipate this result even before all the hard calculations of this section. As we just showed in section 3.2.1, all quadratic parent Hamiltonians of a two band system must be in the form $h(k_x, k_y) = \frac{\varepsilon(k_x, k_y)}{2} g(k_x, k_y)$. Secondly we note that the proportionality factor between the two matrices, except for an irrelevant constant, is exactly the determinant $q(k_x, k_y)$. From the discussion in section 3.2.3, we could almost expected such a behaviour: $\varepsilon(k_x, k_y) \propto q(k_x, k_y)$ is the only way to get rid of the singularity in the hopping terms $h(k_x, k_y)$ that would have precluded the locality of \hat{H} . But, since the above construction of the parent Hamiltonian guarantees its locality, the cancellation of the singularity was unavoidable, as indeed it has happened.

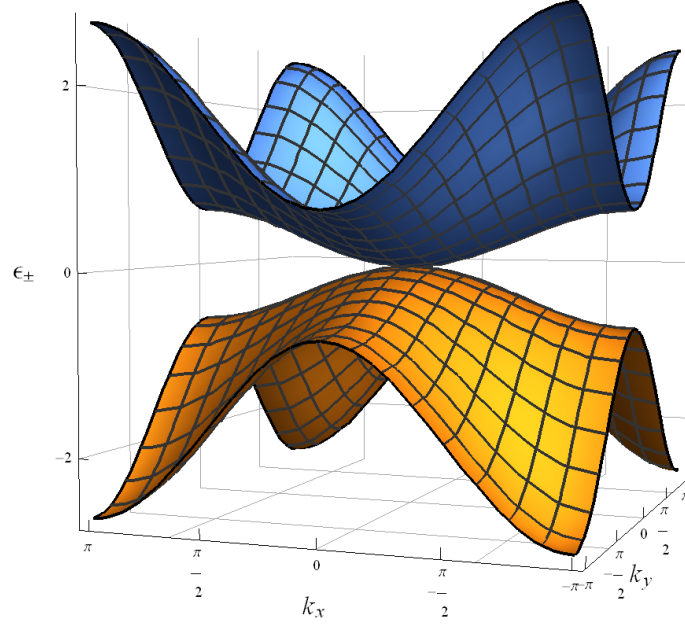


Figure 5.1: Single-particle energy spectrum of \hat{H} . The band-touching point is at $k = (0, 0)$.

5.3 Perturbation of the local parent Hamiltonian

In this section we try to perturb the local gapless parent Hamiltonian found in the previous section. The first aim is to understand if our GFPEPS can be actually the state describing a quantum phase transition between different topological phases identified by a Chern number C . To properly define the Chern number we need a gapped system in order to compute C for the lowest occupied band. We propose the following local perturbation depending on two parameters, μ and ν .

$$\hat{H}' = \hat{H} + \delta\hat{H}(\mu, \nu), \quad (5.12)$$

with

$$\delta\hat{H}(\mu, \nu) = 2i\mu \sum_r \hat{c}_r^1 \hat{c}_r^2 + i\nu \sum_r (\hat{c}_{r+\hat{x}}^1 \hat{c}_r^2 + \hat{c}_{r+\hat{y}}^1 \hat{c}_r^2 - \hat{c}_r^1 \hat{c}_{r+\hat{x}}^2 - \hat{c}_r^1 \hat{c}_{r+\hat{y}}^2). \quad (5.13)$$

The first term is an on-site interaction: since $i\hat{c}_r^1 \hat{c}_r^2 = \hat{a}_r \hat{a}_r^\dagger - \hat{a}_r^\dagger \hat{a}_r = \mathbb{1} - 2\hat{N}_r$, for $\mu > 0$ the interaction encourages the presence of an electron for each site. The second term is instead an hopping term between neighbouring sites. In terms of the matrix of coefficients,

$\delta\hat{H}(\mu, \nu)$ reads

$$\begin{aligned} \delta H(\mu, \nu)_{rs} = & \mu \delta_{rs} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \\ & + \frac{\nu}{2} \begin{pmatrix} 0 & \delta_{r+\hat{x},s} + \delta_{r+\hat{y},s} - \delta_{r,s+\hat{x}} - \delta_{r,s+\hat{y}} \\ \delta_{r+\hat{x},s} + \delta_{r+\hat{y},s} - \delta_{r,s+\hat{x}} - \delta_{r,s+\hat{y}} & 0 \end{pmatrix}. \end{aligned} \quad (5.14)$$

Notice that $\delta H(\mu, \nu)$ is antisymmetric in the simultaneous exchange of mode index and space index: the first term is symmetric in space and antisymmetric for the modes, vice versa for the second term. From this matrix we can go to Fourier space, obtaining

$$\delta h(\mu, \nu, k_x, k_y) = \begin{pmatrix} 0 & -\mu + i\nu(\sin k_x + \sin k_y) \\ \mu + i\nu(\sin k_x + \sin k_y) & 0 \end{pmatrix} \quad (5.15)$$

or, in terms of real components:

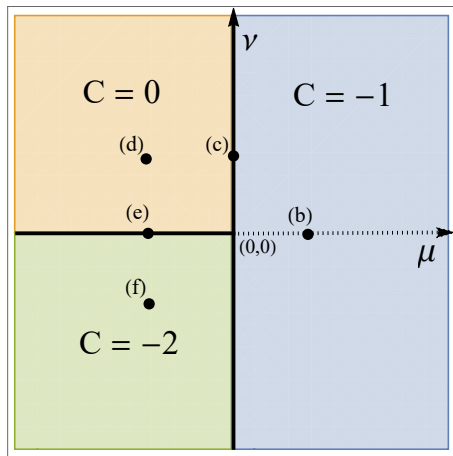
$$\begin{aligned} \delta h^1(\mu, \nu, k_x, k_y) &= \nu(\sin k_x + \sin k_y), \\ \delta h^2(\mu, \nu, k_x, k_y) &= -\mu, \\ \delta h^3(\mu, \nu, k_x, k_y) &= 0. \end{aligned} \quad (5.16)$$

The ground state of this perturbed Hamiltonian will be a gaussian state, since the perturbation is still quadratic. The ground state and the energy are given by (3.70). In particular, the energy $\epsilon(k)$ of the lower band is given by

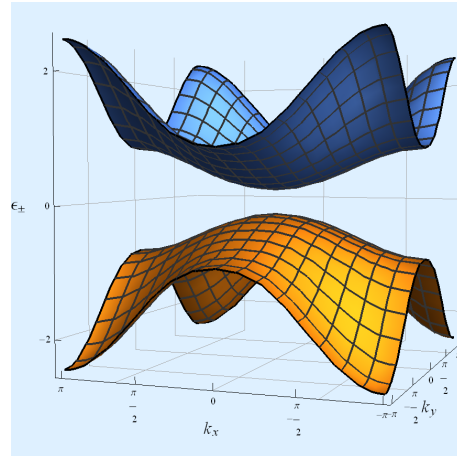
$$\begin{aligned} \epsilon'(k) = -\epsilon'(k) &= -2 \sqrt{\sum_i h^i(k)^2} \\ &= -2 \sqrt{\sum_i (h^i(k)^2 + 2\delta h^i(\mu, \nu, k)h^i(k) + \delta h^i(\mu, \nu, k)^2)} \\ &= -\sqrt{\epsilon(k)^2 + 8 \sum_i \delta h^i(\mu, \nu, k)h^i(k) + 4 \sum_i \delta h^i(\mu, \nu, k)^2}. \end{aligned} \quad (5.17)$$

Since the energy spectrum is given by $\pm\epsilon(k)$, we would like to understand whether the two bands are touching for some k or not, leading to a gapless or gapped system. We consider now only small perturbation in μ and ν . As can be shown, (fig. 5.2), the new Hamiltonian is gapped almost for every choice of parameters, except for $\mu = 0$ and $\nu = 0$, $\mu \leq 0$. We obtain then the following phase diagram in the space of parameters μ and ν divided in regions by the lines of gapless Hamiltonians. We can expect also different Chern numbers that distinguish these regions. The Chern number is computed by (4.49).

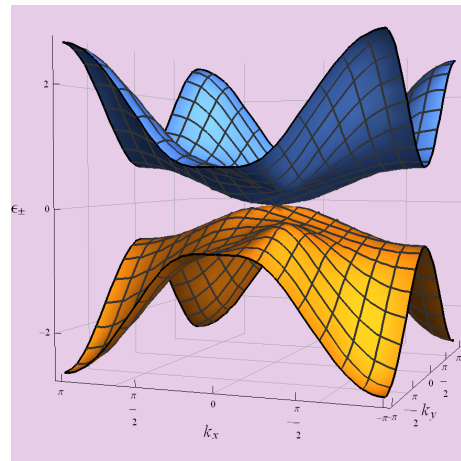
We can conclude that the frustration-free Hamiltonian of our starting GFPEPS is gapless and thus not topologically protected. Instead, it is at the critical point between free-fermionic topological phases with different Chern numbers.



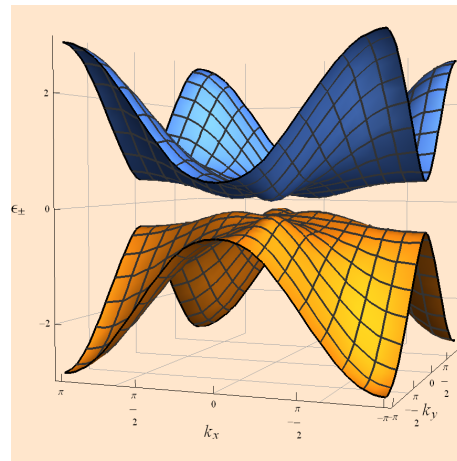
(a) Phase diagram of the perturbed Hamiltonian $\hat{H}(\mu, \nu)$; continuum lines correspond to gapless Hamiltonians.



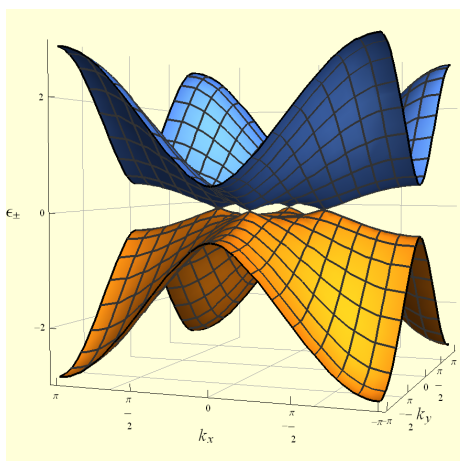
(b) $\mu > 0, \nu = 0$, open gap



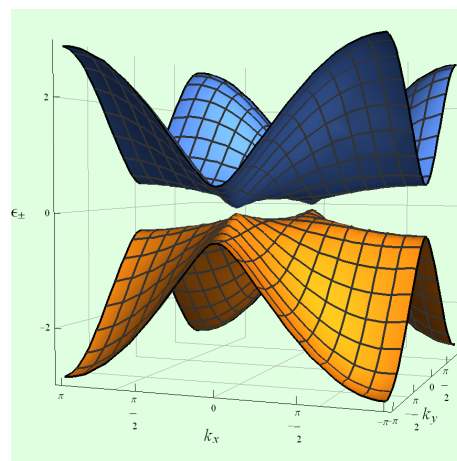
(c) $\mu = 0, \nu > 0$, close gap



(d) $\mu < 0, \nu > 0$, open gap



(e) $\mu < 0, \nu = 0$, close gap



(f) $\mu < 0, \nu < 0$, open gap

Figure 5.2: Phase diagram of the perturbed Hamiltonian (μ and ν close to 0) and spectra in different point of the diagram.

5.3.1 Perturbed GFPEPS

In this section we would like to understand whether it is possible to rewrite the ground state of the perturbed Hamiltonian as a GFPEPS. The answer is immediate: as we showed in section 3.2.2, to be a GFPEPS, the components $g^i(k)$ should be fraction of finite-degree trigonometric polynomial. Since, from (3.70), $g^i(k) = \frac{h^i(k)}{2\varepsilon^i(k)}$, the only possibility is that $\varepsilon^i(k)$ is a trigonometric finite-degree polynomial. However, as can be easily seen from (5.17), the terms under the square root cannot be put in the form of the square of a trigonometric polynomial. What remains is the square root of a trigonometric polynomial that is not what we hoped.

Nevertheless, we can try to approximate the new ground state by a GFPEPS only at first order of the perturbation. From (5.17), the first order in $\delta \sim \mu \sim \nu$ reads

$$\varepsilon'(k) = \varepsilon(k) \left(1 + \frac{4 \sum_i \delta h^i(\mu, \nu, k) h^i(k)}{\varepsilon(k)^2} \right) + \mathcal{O}(\delta^2), \quad (5.18)$$

then, at first order, the 2×2 matrix $g'(k)$ is

$$g'(k) = \frac{h'(k)}{2\varepsilon'(k)} = g(k) + \frac{1}{2\varepsilon(k)} \left(\delta h(k, \mu, \nu) - \frac{4h(k)}{\varepsilon(k)^2} \sum_i \delta h^i(\mu, \nu, k) h^i(k) \right) + \mathcal{O}(\delta^2). \quad (5.19)$$

We define

$$\delta g(k) := \frac{1}{2\varepsilon(k)} \left(\delta h(k, \mu, \nu) - \frac{4h(k)}{\varepsilon(k)^2} \sum_i \delta h^i(\mu, \nu, k) h^i(k) \right) \quad (5.20)$$

Perturbation of the correlation matrix

To find the GFPEPS that at first order may describe $g'(k)$, we should first make a perturbation on the gaussian fiducial state, in a way that the new state is still gaussian. Since the entire information of the fiducial state is contained in the correlation matrix, perturbing the fiducial state corresponds to perturbing M :

$$M' = M + \delta M \quad (5.21)$$

in a way that the new M' still satisfies the requirements for the correlation matrix of a pure state, namely

$$M'^T M' = \mathbb{1}, \quad M'^T = -M'. \quad (5.22)$$

To satisfies these requirements, at first order we just need to impose

$$M\delta M + \delta M M = 0, \quad \delta M^T = -\delta M \quad (5.23)$$

for the matrix δM . Once properly parametrized δM , the aim is to find it such that it gives $g'(k)$ at first order from the formula (3.90). Keeping only the first order and remembering the the zero-th order is already satisfied by the initial $g(k)$, this formula becomes

$$\begin{aligned} \delta g(k) = & \delta A + \delta B(D + \gamma(k))^{-1} B^T + B(D + \gamma(k))^{-1} \delta B^T \\ & - B(D + \gamma(k))^{-1} \delta D (D + \gamma(k))^{-1} B^T \end{aligned} \quad (5.24)$$

that it is formally obtained differentiating (3.90)¹. The matrices $\delta A, \delta B, \delta D$ are the blocks of δM

$$\delta M = \begin{pmatrix} \delta A & \delta B \\ -\delta B^T & \delta D \end{pmatrix} \quad (5.27)$$

that we would like to find in order to satisfy (5.24).

We tried to solve the above equation numerically. We notice, however, that it is quite hard that it can be satisfied since it must hold for every k (discrete, we don't necessarily require a GFPEPS in the thermodynamic limit). One possibility to approach the problem in a more hopeful way would be increasing the bond dimension of the GFPEPS, namely increasing the number of virtual layer. This case will be discussed in the next section.

Here we give some other brief details on how we can set up the problem numerically, keeping the number of virtual layer $\chi = 1$, as above. (5.24) is a system of linear equations, precisely three equations (the number of independent components of $\delta g(k)$) for each k . The variables are the entries of $\delta A, \delta B$ and δD , that must be constrained by (5.23). To make the constraints explicitly, we block diagonalized M by an orthogonal matrix O (this can always be done as long as M is antisymmetric) in 2×2 blocks. From the orthogonality condition, this blocks are all in the form

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad (5.28)$$

and then

$$\Lambda := O^T M O = \begin{pmatrix} 0 & 1 & & & & \\ -1 & 0 & & & & \\ & & 0 & 1 & & \\ & & -1 & 0 & & \\ & & & & 0 & 1 \\ & & & & -1 & 0 \end{pmatrix}. \quad (5.29)$$

If we define $\delta \Lambda := O^T \delta M O$, it is not hard to see that the constraints (5.23) for $\delta \Lambda$ becomes

$$\delta \Lambda = \begin{pmatrix} 0 & 0 & a & b & c & d \\ 0 & 0 & b & -a & d & -c \\ -a & -b & 0 & 0 & e & f \\ -b & a & 0 & 0 & f & -e \\ -c & -d & -e & -f & 0 & 0 \\ -d & c & -f & e & 0 & 0 \end{pmatrix} \quad (5.30)$$

¹In particular, to compute the differential $\delta(D + \gamma(k))^{-1} = (D + \delta D + \gamma(k))^{-1} - (D + \gamma(k))^{-1}$ one can use the following trick for generic matrices P (invertible) and Q :

$$(P + Q)^{-1} = P^{-1} - P^{-1}Q(P + Q)^{-1}. \quad (5.25)$$

In particular, calling $P = D + \gamma(k)$ and $Q = \delta D$, at first order we obtain

$$\delta(D + \gamma(k))^{-1} = -(D + \gamma(k))^{-1} \delta D (D + \gamma(k))^{-1}. \quad (5.26)$$

One can also apply the trick iteratively to find the following orders.

We found then the we can play with 6 free parameters in order to solve the system of equations.

As in part expected, the numerical result is disappointing: the equation (5.24) cannot be satisfied for any choice of parameters. Actually, the situation is even worse: (5.24) cannot be satisfied for any k independently (except for $k = (0, 0)$, if we take the limit (5.5) as the definition of $g(0, 0)$ not even in the thermodynamic limit²).

Perturbation with increasing virtual layer

In the very spirit of tensor networks, now we would like to increase the bond dimension of the GFPEPS in order to find the right first order approximation of the gaussian ground state of the perturbed Hamiltonian. We anticipate immediately that even this method happens to fail miserably.

One of the major problem in the previous section was the great number of linear equations that we aim to solve, number that increases N , against the fixed number of parameters in δM . In one dimension, the way to approximate states with increasing N is to increase sufficiently the bond dimension: precisely, for translational invariant systems, ground states of local and gapped Hamiltonians are well described by MPS, in the sense that, increasing N , we just need a bond dimension D that increases polynomially in N in order to approximate the ground state within a certain error. In the GFPEPS formalism, increasing the bond dimension corresponds to increase the number of virtual modes that we allow for each site: we define *virtual layer* to be two virtual fermionic modes, one vertical and the other horizontal, corresponding to four Majorana's modes; until now we always choose one virtual layer $\chi = 1$. The correlation matrix M of the fiducial state then increase from 6×6 to 10×10 , 14×14 ... More generally, with f physical fermionic modes and χ virtual layers, M is a $(2f + 4\chi) \times (2f + 4\chi)$ matrix. Anyway, for our system $f = 1$.

To make a perturbation with increased bond dimension, first we need to increase it in the zero-th case. To do this, we should try to find a family of extended correlation matrices \bar{M} $(2 + 4\chi) \times (2 + 4\chi)$ such that they give the same initial GFPEPS $g(k)$ by formula (3.90),

²The case $k = (0, 0)$ is trivially satisfied because $\delta g(0, 0) = 0$ and then we could choose $\delta M = 0$. $\delta g(0, 0) = 0$ is not surprising at all if we consider that a generic 2×2 matrix satisfying (3.55) for $k = (0, 0)$ must be in the form

$$g(0, 0) = \begin{pmatrix} 0 & \pm 1 \\ \mp 1 & 0 \end{pmatrix}. \quad (5.31)$$

Since we require continuity between $g(0, 0)$ and $g'(0, 0)$ varying the perturbing parameters μ and ν , they must be equal.

valid also for $\chi > 1$ ³. We parametrize \bar{M} as

$$\bar{M} = \begin{pmatrix} \bar{A} & \bar{B}_1 & \bar{B}_2 \\ -\bar{B}_1^T & \bar{D}_1 & \bar{D}_2 \\ -\bar{B}_2^T & -\bar{D}_2^T & \bar{D}_3 \end{pmatrix}, \quad (5.34)$$

where the up left 2×2 block has dimensions 6×6 , while the extension in the last row has generically $4(\chi - 1)$ rows. In summary, this matrix must be antisymmetric, orthogonal and must give the same GFPEPS $g(k)$ obtained from M . To satisfies these requirements for every k is not hard to see that the only proper way to increase the bond dimension is extending M by placing an orthogonal and antisymmetric matrix O in the lower right corner:

$$\bar{M} = \begin{pmatrix} A & B & 0 \\ -B^T & D & 0 \\ 0 & 0 & O \end{pmatrix}. \quad (5.35)$$

We notice that in this way, the formula (3.90) for \bar{M} give the same $g(k)$; furthermore, \bar{M} is orthogonal and antisymmetric.

We can now set up the perturbation by the following matrix $\delta\bar{M}$:

$$\delta\bar{M} = \begin{pmatrix} \delta A & \delta\bar{\mathbb{B}} \\ -\delta\bar{\mathbb{B}}^T & \delta\bar{\mathbb{D}} \end{pmatrix}. \quad (5.36)$$

We now get the expression that gives $\delta g(k)$: it is the same as in (5.24), but with the

³(3.90) still holds with the correlation matrix $\gamma(k)$ of the projector properly increased: for the new virtual layers we should construct new projectors in analogy with (3.18) and (3.19):

$$\begin{aligned} \hat{\omega}_r^{hn} &:= \frac{1}{2}(\mathbb{1} + i\hat{\gamma}_{r+\hat{x}}^l \hat{\gamma}_r^r), \\ \hat{\omega}_r^{vn} &:= \frac{1}{2}(\mathbb{1} + i\hat{\gamma}_{r+\hat{y}}^u \hat{\gamma}_r^d), \end{aligned} \quad (5.32)$$

where we add a new index $n = 1, \dots, \chi$. The correlation matrix $\bar{\gamma}k$ of the new bigger projector then becomes

$$\bar{\gamma}(k) = \bigoplus_{n=1}^{\chi} \gamma(k), \quad (5.33)$$

where γk is the correlation matrix (3.87).

extended matrices.

$$\begin{aligned}
\delta g(k) &= \delta A + \delta \bar{\mathbb{B}} \begin{pmatrix} (D + \gamma(k))^{-1} & 0 \\ 0 & (O + \gamma(k))^{-1} \end{pmatrix} \begin{pmatrix} -B^T \\ 0 \end{pmatrix} \\
&+ (B \ 0) \begin{pmatrix} (D + \gamma(k))^{-1} & 0 \\ 0 & (O + \gamma(k))^{-1} \end{pmatrix} \delta \bar{\mathbb{B}} \\
&- (B \ 0) \begin{pmatrix} (D + \gamma(k))^{-1} & 0 \\ 0 & (O + \gamma(k))^{-1} \end{pmatrix} \delta \bar{\mathbb{D}} \\
&\qquad \qquad \qquad \begin{pmatrix} (D + \gamma(k))^{-1} & 0 \\ 0 & (O + \gamma(k))^{-1} \end{pmatrix} \begin{pmatrix} -B^T \\ 0 \end{pmatrix} \\
&= \delta A + \delta B(D + \gamma(k))^{-1}B^T + B(D + \gamma(k))^{-1}\delta B^T \\
&\quad - B(D + \gamma(k))^{-1}\delta D(D + \gamma(k))^{-1}B^T.
\end{aligned} \tag{5.37}$$

As one can notice, we wanted to increase the bond dimension to increase the number of parameters in order to recover $\delta g(k)$, but it happens that the new degrees of freedom in $\delta \bar{M}$ do not enter in the expression above due to the presence of the zeros in (5.35).

We conclude that, by increasing the bond dimension, the equation for $\delta g(k)$ does not change at first order. This rules out definitely the possibility of approximating the new chiral ground state of the gapped Hamiltonian with a gaussian fermionic PEPS at first order. We leave some other possible approaches in the Outlook.

Chapter 6

Conclusions and Outlook

At the end, the conclusion of this work is an impossibility result that cast further doubts on the possibility of describing chiral systems by GFPEPS. We summarize the main results we got.

- As we showed in section 4.2, we cannot have topological, in particular chiral, injective GFPEPS. Together with the strong belief that injective PEPS are ground states of local and gapped Hamiltonians, we conclude that we cannot have a chiral GFPEPS that is ground state of local and gapped Hamiltonians.
- Chapter 5 showed that, at least in our model, starting from a GFPEPS on a phase transition and perturbing quadratically the Hamiltonian in a gapped topological phase leads to a ground state that cannot be described by a GFPEPS, neither at the first perturbative order. We remark the fact that, from the previous point, we did not expect a GFPEPS for the perturbed ground state, but at least a GFPEPS (non chiral) that is equal to the ground state at some orders in the perturbation.
- Actually in chapter 5 we obtained an other parallel result: whenever we perturb the fiducial state of a GFPEPS, maintaining its gaussianity but allowing an higher bond dimension, the new GFPEPS happens to be independent on the the new bond dimension at first order in the perturbation. Then, the bond dimension does not influence the perturbation at first order.

Nevertheless, it was shown [19] that GFPEPS can be used numerically to approximate chiral free fermionic systems in gapped phases with a small bond dimension. However, it is almost clear that the complete physics of these states can never be stored in a GFPEPS. This is analogous to MPS of small bond dimension that can be used to study critical system [15].

There can be further possibilities left open in the study of the model in chapter 5, in particular one can allow a description of chiral free fermionic systems by FPEPS that are not GFPEPS.

- In the perturbative framework of chapter 5, a possible new attempt would be to find a FPEPS that is gaussian only at first order but loses gaussianity at higher orders.

In this way, one could find a quasi-gaussian FPEPS that is near the chiral topological ground state: then one should compute the Chern number of the FPEPS and find out if the FPEPS is trivial or not. Unfortunately, in this framework, the formalism we developed with correlation matrices is no more usable: this approach should be investigated numerically.

- However, there is one more tight possibility. We remark the fact that, by a quadratic perturbation, the ground state of the new Hamiltonian is still gaussian. Furthermore, in the definition of GFPEPS given in 3.2.2, we imposed that the fiducial state was gaussian, not the GFPEPS itself. Nevertheless, we showed that the GFPEPS obtained from a gaussian fiducial state is actually gaussian. A natural question arises. Is every FPEPS that happens to be a gaussian state a GFPEPS? Indeed, it is not clear whether starting from a non-gaussian fiducial state we can end with a FPEPS that is gaussian. This would be a good possibility because we investigate in a larger class of FPEPS and maybe be able to find chiral FPEPS that are ground states of free fermionic gapped Hamiltonians.

Appendix A

Quantum information tools

A.1 Schmidt Theorem

The *Schmidt theorem* allows to write in a very compact representation a quantum state living in a bipartite system AB . At the basis of this theorem there is the *singular value decomposition* that guarantees for an arbitrary complex rectangular matrix M of dimensions $n \times m$ (let's suppose $n \leq m$) the existence of the decomposition

$$M = UDV^\dagger, \tag{A.1}$$

where

- U of dimension $n \times n$ is a unitary matrix: $U^\dagger U = \mathbb{1}$;
- D of dimension $n \times n$ is a diagonal matrix with real and non-negative entries; the number r of positive values is called *Schmidt rank of M* ;
- V of dimension $m \times n$ is a matrix with orthonormal columns, i.e. $V^\dagger V = \mathbb{1}$.

The Schmidt theorem is a corollary of the singular value decomposition and states that, given a quantum state $|\psi\rangle$ in an Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ (with $n = \dim \mathcal{H}_A$, $m = \dim \mathcal{H}_B$ and $n \leq m$), it can be always decomposed on the given bipartition as

$$|\psi\rangle = \sum_{i=1}^r \lambda_i |\phi_i\rangle |\tilde{\phi}_i\rangle,$$

where $r < n$, $\{|\phi_i\rangle\}_{i=1}^r \subseteq \mathcal{H}_A$ and $\{|\tilde{\phi}_i\rangle\}_{i=1}^r \subseteq \mathcal{H}_B$ are orthonormal sets in the two Hilbert spaces and λ_i are real and positive numbers uniquely determined by $|\psi\rangle$. The coefficients λ_i are called *Schmidt coefficients* and their number r is called *Schmidt number* or *Schmidt rank* of $|\psi\rangle$.

Clearly, a pure state is separable if and only if its Schmidt rank is equal to 1 and then its only Schmidt coefficient is 1 by normalization, i.e. $|\psi\rangle = |\phi\rangle |\tilde{\phi}\rangle$.

A.2 Entanglement measures

We introduce a measure that quantifies the entanglement of a state or, better, the grade of entanglement between the two subsystems of a bipartition of the state. To achieve this aim, we use the *Von Neumann entropy*, a quantity that indicates the entropy of a mixed state described by a density matrix ρ :

$$S(\rho) := -\text{Tr}(\rho \ln \rho). \quad (\text{A.2})$$

If we diagonalize the matrix ρ obtaining the eigenvalues $1 \geq p_i > 0$, $i = 1, \dots, \text{rk}(\rho)$, it is easy to see that $S(\rho) = -\sum_i p_i \log p_i$. Therefore, $S(\rho)$ satisfies some usual properties for an entropy, namely it is always non-negative, it is zero if ρ is actually a pure state, it is invariant under a change of basis $U\rho U^\dagger$, it is concave in ρ and it is additive in independent systems (i.e. if $\rho = \rho_A \otimes \rho_B$, meaning that the two systems do not interact, $S(\rho) = S(\rho_A) + S(\rho_B)$). Furthermore, its maximum value is reached when all the probabilities p_i are equal to $\frac{1}{\text{rk}(\rho)}$, then $S(\rho) \leq \log \text{rk}(\rho)$. In the case of a system in the Hilbert space $(\mathbb{C}^d)^{\otimes L}$, for example a lattice with L sites and a d -dimensional spin per site, the maximum possible rank is given by d^L , then we have $S(\rho) \leq L \log d$.

Actually, we could also define another family of measures of entropy in a quantum state given by the *Rényi entropy*:

$$S_\alpha(\rho) := \frac{1}{1-\alpha} \ln \text{Tr}(\rho^\alpha), \quad (\text{A.3})$$

with $\alpha \geq 0$. This quantity reduces to the Von Neumann entropy in the limit $\alpha \rightarrow 1^+$. It can be proven also that S_α is not increasing in α .

We now define a proper measure for entanglement. Given a state $|\psi\rangle$ we define the *Von Neumann entanglement entropy* to quantify the entanglement between a bipartition of this state: it is simply the Von Neumann entropy computed on either the reduced states of the bipartition $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. Defining $\rho = |\psi\rangle\langle\psi|$, $\rho_A = \text{Tr}_B(\rho)$ and $\rho_B = \text{Tr}_A(\rho)$ this measure of entanglement is given by

$$S(\rho_A) = -\text{Tr}(\rho_A \ln \rho_A) = -\text{Tr}(\rho_B \ln \rho_B) = S(\rho_B). \quad (\text{A.4})$$

We notice in particular that if the state has not entanglement between its constituents, i.e. the state is separable ($|\psi\rangle = |\phi\rangle_A \otimes |\phi\rangle_B$), the above expression gives 0, consistently.

Similarly, one can define a *Rényi entanglement entropy* starting from the Rényi entropy.

Appendix B

Grassmann Algebra

To deal with gaussian formalism for fermions in an efficient way, we will largely use anticommuting variables, precisely the Grassmann algebra [4]. A *Grassmann algebra* (\mathcal{G}_n) is an algebra over the complex field generated by $\theta_1, \dots, \theta_n$ (considered as abstract elements) with the following constraint:

$$\{\theta_a, \theta_b\} = 0.$$

In particular, we notice that $\theta_a^2 = 0$. An arbitrary element $f(\theta) \in \mathcal{G}_n$ can be written as

$$f(\theta) = \alpha + \sum_{p=1}^n \sum_{1 \leq a_1 < \dots < a_p \leq n} \alpha_{a_1, \dots, a_p} \theta_{a_1} \cdots \theta_{a_p}$$

with $\alpha, \alpha_{a_1, \dots, a_p} \in \mathbb{C}$ ¹. We notice also that even polynomials of θ (such as $\theta_1\theta_2$, $\theta_1\theta_3\theta_4\theta_5 + 1 + 3\theta_2\theta_3$, but not, for example, θ_1 and $\theta_1\theta_2\theta_3 - \theta_1\theta_2$) commute with the whole algebra, i.e. they constitute the *center* of the Grassmann algebra.

Now we introduce some calculus on this algebra. First we define the partial derivative $\frac{\partial}{\partial \theta_a} : \mathcal{G}_n \rightarrow \mathcal{G}_n$ that follows some basic rules:

- $\frac{\partial}{\partial \theta_a} 1 = 0$,
- $\frac{\partial}{\partial \theta_a} \theta_b = \delta_{ab}$,
- (*Anticommuting Leibniz's rule*)

$$\frac{\partial}{\partial \theta_a} (\theta_b f) = \delta_{ab} f - \theta_b \frac{\partial}{\partial \theta_a} f \tag{B.1}$$

¹Strictly speaking we have not defined the sum between an element generated by $\theta_1, \dots, \theta_n$ and a scalar α . In general, given an algebra \mathcal{A} over the field \mathbb{K} , \mathcal{A} can be extended to an unital algebra $\tilde{\mathcal{A}}$, i.e. an algebra with an element $\mathbb{1}$ such that $a\mathbb{1} = \mathbb{1}a = a, \forall a \in \tilde{\mathcal{A}}$. The extension can be performed defining $\tilde{\mathcal{A}} := \mathbb{K} \oplus \mathcal{A}$, where \oplus is the direct product with the sum defined as in the direct product between vectorial spaces and the product given by $(\lambda, a)(\mu, b) = (\lambda\mu, \lambda b + \mu a + ab)$. The unit element is then $(1, 0)$. Finally we can forget the parenthesis and identify $(\lambda, a) \equiv \lambda + a$.

From this properties, it follows that the derivatives anticommutes

$$\left\{ \frac{\partial}{\partial \theta_a}, \frac{\partial}{\partial \theta_b} \right\} = 0. \quad (\text{B.2})$$

Furthermore, we define the integration to have the same effect of the derivation

$$\int d\theta_a := \frac{\partial}{\partial \theta_a}. \quad (\text{B.3})$$

We will also use the notation

$$\int D\theta := \int d\theta_n \cdots \int d\theta_1. \quad (\text{B.4})$$

With this order we have that $\int D\theta \theta_1 \cdots \theta_n = 1$. From the anticommutation relation [B.2](#) it follows that

$$\int D\theta \frac{\partial}{\partial \theta_a} f(\theta) = 0 \quad (\text{B.5})$$

so from the Leibniz rule [B.1](#) we can use the anticommuting version of integration by parts:

$$\int D\theta g(\theta) \frac{\partial f}{\partial \theta_a}(\theta) = \int D\theta \frac{\partial g}{\partial \theta_a}(\theta) f(\theta). \quad (\text{B.6})$$

From now on we will consider only even-dimensional Grassmann algebras \mathcal{G}_{2n} . We will usually need quadratic forms in the Grassmann Algebra to work with gaussian states. We will denote a quadratic form by

$$\theta^T M \theta = \sum_{a=1}^{2n} M_{ab} \theta_a \theta_b \in \mathcal{G}_{2n}, \quad (\text{B.7})$$

where M is a real and antisymmetric matrix $2n \times 2n$. Finally, we present two formulas for Gaussian integrals that we shall extensively use:

$$\int D\theta e^{\pm \frac{i}{2} \theta^T M \theta} = \pm i^n \text{Pf}(M), \quad (\text{B.8})$$

$$\int D\theta e^{(i)^\alpha \eta^T \theta \pm \frac{i}{2} \theta^T M \theta} = \pm i^n \text{Pf}(M) e^{\pm (-1)^\alpha \frac{i}{2} \eta^T M^{-1} \eta}, \quad (\text{B.9})$$

where $\text{Pf}(M)$ is the Pfaffian of the matrix M defined as

$$\text{Pf}(M) = \frac{1}{2^n n!} \sum_{\sigma \in S_{2n}} \text{sgn}(\sigma) M_{\sigma_1, \sigma_2} \cdots M_{\sigma_{2n-1}, \sigma_{2n}}. \quad (\text{B.10})$$

Appendix C

Fourier transform: smoothness and decay

We present here some results about the Fourier transform in one dimension [8] [16]. These results are generalizable also for two-dimensions.

We consider a function $f(x) \in \mathcal{L}^2(\mathbb{R})$ with Fourier transform given by

$$\hat{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-ikx} f(x) dx. \quad (\text{C.1})$$

Also $\hat{f}(k) \in \mathcal{L}^2(\mathbb{R})$. From $\hat{f}(k)$ we can recover $f(x)$ by

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{ikx} \hat{f}(k) dx. \quad (\text{C.2})$$

The following propositions hold:

- $\hat{f}(k)$ has $p - 1$ continuous derivatives in $\mathcal{L}^2(\mathbb{R})$ for some $p \geq 0$ and the p th derivative in $\mathcal{L}^2(\mathbb{R})$ with bounded variation¹ if and only if

$$f(x) = \mathcal{O}(|x|^{-p-1}) \text{ as } |x| \rightarrow \infty; \quad (\text{C.3})$$

- $\hat{f}(k)$ has infinitely many continuous derivatives in $\mathcal{L}^2(\mathbb{R})$ if and only if

$$\forall M, f(x) = \mathcal{O}(|x|^{-M}) \text{ as } |x| \rightarrow \infty. \quad (\text{C.4})$$

¹A function $g(x)$ on \mathbb{R} is said to have *bounded variation* if there is a constant M such that for any finite m and any points $x_0 < x_1 < \dots < x_m$, $\sum_{j=1}^m |g(x_j) - g(x_{j-1})| < M$.

Appendix D

Complete formulas for the family of GFPEPS

We summarize here a slight generalization of the model in chapter 5 [20], involving a more general family of GFPEPS parametrized by λ . All the properties of these GFPEPS are equivalent to the case discussed in 5, that corresponds to the case $\lambda = \frac{1}{2}$.

$$\begin{aligned}
 A &= \begin{pmatrix} 0 & 1-2\lambda \\ -1+2\lambda & 0 \end{pmatrix}, \\
 B &= \sqrt{\lambda-\lambda^2} \begin{pmatrix} 1 & -1 & 0 & -\sqrt{2} \\ -1 & -1 & -\sqrt{2} & 0 \end{pmatrix}, \\
 D &= \begin{pmatrix} 0 & 1-\lambda & -\frac{\lambda}{\sqrt{2}} & -\frac{\lambda}{\sqrt{2}} \\ -1+\lambda & 0 & \frac{\lambda}{\sqrt{2}} & -\frac{\lambda}{\sqrt{2}} \\ \frac{\lambda}{\sqrt{2}} & -\frac{\lambda}{\sqrt{2}} & 0 & 1-\lambda \\ \frac{\lambda}{\sqrt{2}} & \frac{\lambda}{\sqrt{2}} & -1+\lambda & 0 \end{pmatrix};
 \end{aligned} \tag{D.1}$$

$$\hat{\phi}_r^\dagger = \sqrt{1-\lambda} \mathbb{1} + \sqrt{\frac{\lambda}{2}} e^{-i\frac{\pi}{4}} \hat{a}_r^\dagger \hat{h}_r^\dagger + \sqrt{\frac{\lambda}{2}} \hat{a}_r^\dagger \hat{v}_r^\dagger; \tag{D.2}$$

$$q(k_x, k_y) = 2(2-4\lambda+3\lambda^2-2(1-\lambda)^2(\cos k_x + \cos k_y) + (2-4\lambda+\lambda^2) \cos k_x \cos k_y); \tag{D.3}$$

$$\begin{aligned}
 g^1(k_x, k_y) &= -\frac{8(1-\lambda)\lambda}{q(\lambda, k_x, k_y)} \sin^2 \frac{k_x}{2} \sin k_y, \\
 g^2(k_x, k_y) &= \frac{2}{q(\lambda, k_x, k_y)} (2-4\lambda+\lambda^2-2(1-\lambda)^2(\cos k_x + \cos k_y) \\
 &\quad + (2-4\lambda+3\lambda^2) \cos k_x \cos k_y), \\
 g^3(k_x, k_y) &= \frac{8(1-\lambda)\lambda}{q(\lambda, k_x, k_y)} \sin k_x \sin^2 \frac{k_y}{2}.
 \end{aligned} \tag{D.4}$$

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