Master Thesis

Impurity Bound States
in Variants of the Kitaev Spin Liquid

Hugo Théveniaut

Condensed Matter Physics, Department of Theoretical Physics,
School of Engineering Sciences
Royal Institute of Technology, SE-106 91 Stockholm, Sweden

Stockholm, Sweden 2017
Scientific thesis for the degree of Master of Engineering in the subject area of Theoretical physics.

TRITA-FYS 2017:19
ISSN 0280-316X
ISRN KTH/FYS/--17:19SE

© Hugo Théveniaut, March 2017
Printed in Sweden by Universitetsservice US AB, Stockholm March 2017
Abstract

The recent developments of topological quantum computing have brought about a lot of new challenges in the field of condensed matter physics. In particular, after the seminal paper of Alexei Kitaev [2], research has been focused on the realisation of such computers implemented by Majorana fermions. The manipulation of such unusual particles as the new "qubits" requires good localization and non-abelian exchange statistics. This is achieved if these bound states arise in spectral gaps and are coupled to fluxes.

The main purpose of this thesis is to study the formation of bound states in the Kitaev honeycomb lattice model and its variants. We find that no such states can arise in the gapped phase of the Kitaev model. However, more satisfactory results occur when a distorted version of the Kitaev model is considered. In this case, the insertion of impurities can produce clear localized in-gap states.

Keywords: Kitaev model, Majorana bound states, Kekulé distortion.
Acknowledgements

First and foremost, I would like to thank Matthias Vojta my supervisor in Dresden for giving me the opportunity to work with him on this thesis, for valuable guidance and discussions. I would also like to thank Egor Babaev for having brought my attention to the Institute of Theoretical Physics of Dresden, his advice gave me the chance to experience a rich master thesis.

I would like to thank a lot Chris, Sebastian, Laura and my other colleagues at the Institute of Theoretical Physics at TUD for welcoming me among them.

Finally my thanks go to Santanu, Urban, Erik, Vincent and Laura, my colleagues and flatmates with whom I shared much of my six months in Germany, inside and outside university.
Contents

Abstract ................................................................. iii

Acknowledgements ------------------------------------------ v

Contents vii

Introduction ix

1 Kitaev’s honeycomb lattice model .................................. 1
  1.1 The model ................................................................ 1
  1.2 Exact solution ......................................................... 2
    1.2.1 Conservation laws .......................................... 3
    1.2.2 Majorana representation ................................. 3
    1.2.3 Application to the model ............................... 4
  1.3 Properties of the ground state ................................. 6

2 Impurities in the Kitaev model .................................... 9
  2.1 Scattering theory .................................................. 9
    2.1.1 The bond impurity .................................... 10
    2.1.2 The Lippmann-Schwinger equation ................. 11
    2.1.3 Adapting the $T$-matrix method .................. 11
    2.1.4 Expressions for the Green’s functions .......... 12
  2.2 Detecting the bound states .................................... 13
    2.2.1 Necessary and sufficient conditions for bound states . 13
    2.2.2 Numerical results .................................. 14

3 Kekulé distortion in the Kitaev model ......................... 17
  3.1 The Kekulé distortion ......................................... 18
    3.1.1 Analogy to the Peierls distortion ............... 18
  3.2 Energy spectrum for $\kappa < 1$ .............................. 20
    3.2.1 Behaviour close to $\kappa = 1$ ....................... 21
    3.2.2 Behaviour close to $\kappa = 0$ ....................... 21
    3.2.3 Behaviour in the bulk .............................. 23
  3.3 Energy spectrum for $\kappa > 1$ .............................. 23
3.3.1 Behaviour close to $\kappa = +\infty$ .................................. 24
3.4 Distortion and anisotropic couplings ................................. 25

4 Impurities in the Kekulé-disorted Kitaev model .................... 27
4.1 Response to the impurities .............................................. 27
4.1.1 Numerical results .................................................. 28
4.1.2 Analysis of the bound states energies .......................... 30
4.1.3 Wavefunctions of the in-gap states ......................... 31
4.2 Bound-state spectroscopy .............................................. 32
4.2.1 Dynamic spin structure factor ................................. 32
4.2.2 Numerical results .................................................. 33
4.3 Discussion and outlook ............................................... 34

A Boundary conditions .................................................... 37
A.1 Different types of boundary conditions ......................... 37
A.2 Translation invariance and disorder .......................... 37
A.3 Numerical efficiency and other subtleties .................. 38

Bibliography ................................................................ 39
Introduction

As the components of computers become smaller and smaller, we are approaching the limit in which quantum effects become important. One might ask whether this is a problem or an opportunity. The founders of the field of quantum computation - Manin, Feynman, Deutsch in the 1980s or Shor in 1990s - answered in favor of the latter. They showed that a computer which operates coherently on quantum states has potentially much greater power than a classical computer. In particular, Feynman showed that certain many-body quantum Hamiltonians could be simulated exponentially faster on a quantum computer than they could be on a classical computer.

In 1994, Peter Shor found an application of a quantum computer which generated widespread interest not just inside but also outside of the physics community [3]. He invented an algorithm by which a quantum computer could find the prime factors of an $m$ digit number in a length of time $\sim m^2 \log m \log \log m$. This is much faster than the fastest known algorithm for a classical computer, which takes $\sim \exp(m^{1/3})$ time. Since many encryption algorithm depend on the difficulty of finding the solution to problems similar to finding the prime factors of a large number, there is an obvious application of a quantum computer which is of great basic and applied interest.

Typically the fundamental piece of a quantum computer is taken to be a quantum two state system known as a ”qubit” which is the quantum analogue of a bit. While a classical bit can be either ”zero” or ”one” at any given time, a qubit can be in one of the infinitely many superposition of states $a|0\rangle + b|1\rangle$. Nevertheless the biggest obstacle to building a practical quantum computer is posed by errors. With a quantum computer, the situation is more complex than for its classical counterpart. Indeed, if we measure a quantum state during an intermediate stage of a calculation to see if an error has occurred, we collapse the wave function and thus destroy quantum superpositions and ruin the calculation.

Topological quantum computing is an approach to fault-tolerant quantum computation whose main advantage is that it is robust to localized imperfections. First formulated by Alexei Kitaev [1], this scheme makes use of non-abelian exchange statistics. In order to perform computation in this frame, one needs to create pairs of these non-abelian excitations (called non-abelian anyons) from vacuum, separating them spatially, transporting them around each other to implement the logical gates and finally, fusing them together for measurements.
Anyons are particles with unusual statistics (neither Bose nor Fermi), which can only occur in two dimensions. When two particles interchange along some specified trajectories, the overall quantum state is multiplied by $e^{i\psi}$. In three dimensions, there is only one topologically distinct way to swap two particles. Two swaps are equivalent to the identity transformation, hence $e^{i\psi} = \pm 1$. On the contrary, in two dimensions the double swap corresponds to one particle making a full turn around the other; this process is topologically nontrivial. Therefore the exchange phase $\psi$ can, in principle, have any value - hence the name "anyon".

Overview of the thesis

The main purpose of this thesis is to study localized abelian anyons which can be found for instance in the Kitaev honeycomb lattice model.

To that end, we proceed in the following way. In chapter 1, we review the essential results of the Kitaev honeycomb lattice model. We give a solution of the model and provide an extensive discussion on the properties of the excitations. In chapter 2, we study the effect of an impurity inserted in the lattice. Using the $T$-matrix method, we propose an equation that must be fulfilled by in-gap bound states, possibly arising from the perturbation; we present the numerical results. In chapter 3, we introduce a variant of the Kitaev model where the couplings have been distorted throughout the lattice. This model is studied as a function of the distortion strength. In chapter 4, we analyse the response of the distorted model to the insertion of an impurity and we compute some observables accessible by experiments.
Chapter 1

Kitaev’s honeycomb lattice model

Despite being formulated a decade ago, the Kitaev honeycomb lattice model still holds surprises and the number of recent publications [4, 5, 6] is evidence of the keen interest it still arouses. The reasons of this success are numerous. First and foremost it is one of the exceedingly rare instances of exactly solvable two-dimensional spin Hamiltonians, it is moreover a prime example of a quantum spin liquid (QSL). In fact, the remarkable simplicity of the model has led to a number of proposals for experimental realisations of QSL, the oxides of the family \{Na, L\}_2IrO_3 [7] or more recently \(\alpha\)-RuCl_3 [8] are found to be the most promising candidates. The model is also of great importance regarding the developments of topological quantum computing because of the properties of its ground state and its elementary excitations.

This chapter introduces the model and gives an exact solution. We follow Kitaev’s original approach using Majorana fermions [2]. The phase diagram of the ground state is next discussed.

1.1 The model

The Kitaev model describes ferromagnetically coupled spin-\(\frac{1}{2}\) degrees of freedom localized at the sites of a two-dimensional honeycomb lattice. The spins interact via Ising-like nearest neighbour exchange interactions \(J^\alpha\). The special feature of the model is that the spin components \(\alpha = x, y, z\) are coupled by an exchange that depends on the bond direction. The Hamiltonian reads:

\[
\hat{H}_K = -J^x \sum_{\langle ij \rangle_x} \hat{\sigma}_i^x \hat{\sigma}_j^x - J^y \sum_{\langle ij \rangle_y} \hat{\sigma}_i^y \hat{\sigma}_j^y - J^z \sum_{\langle ij \rangle_z} \hat{\sigma}_i^z \hat{\sigma}_j^z
\]  

(1.1)

where \(\hat{\sigma}_i^\alpha\) are Pauli matrices, and \(\langle ij \rangle_\alpha\) denotes an \(\alpha = x, y, z\) bond as shown in figure 1.1.
Chapter 1. Kitaev’s honeycomb lattice model

This specific type of interaction leads in fact to strong frustration. Indeed, a spin has three preferred orientations that are orthogonal with each other and it is clear that these constraints cannot be fulfilled simultaneously.

Figure 1.1: The honeycomb lattice is shown with its three inequivalent bond directions $x$, $y$ and $z$. The flux operator $\hat{W}_p$, a product of spin operators around a plaquette, is highlighted in red. The elementary unit cell consists of two basis sites $A$ and $B$ (open and full circles) connected by lattice vectors $n_1$ and $n_2$. Figure taken from [9].

1.2 Exact solution

The system being introduced, now we want to find the eigenvalues and eigenvectors of the Kitaev Hamiltonian given in (1.1).

The first step towards the diagonalization of the Hamiltonian $\hat{H}_K$ is to find a common eigenbasis in which the matrix elements can be easily computed. In spin-$\frac{1}{2}$ systems, since the Pauli matrices do not commute with each other, it is often salutary to introduce the ladder operators $\hat{\sigma}^\pm = (\hat{\sigma}^x \pm i\hat{\sigma}^y)$ and the matrix elements can be calculated in the eigenbasis of $\hat{\sigma}^z$. Developing this idea, Jordan and Wigner proposed a transformation allowing to map spin operators onto fermionic operators. The Jordan-Wigner transformation enables a direct solution of the Kitaev model [10], however it assumes translation invariance and consequently is inconvenient to study local defects.

We will follow in this section the original approach of Kitaev [2] representing each spin operator as a product of two Majorana fermions.
1.2. Exact solution

1.2.1 Conservation laws

The solution is made possible thanks to the existence of an extensive number of conserved quantities in the model. In particular, Kitaev introduced for each elementary plaquette of the lattice the operator

$$\hat{W}_p = \hat{\sigma}_1^x \hat{\sigma}_2^y \hat{\sigma}_3^z \hat{\sigma}_4^x \hat{\sigma}_5^y \hat{\sigma}_6^z$$

with $1, \ldots, 6$ labelling the sites of the plaquette $p$ shown in figure 1.1. Remarkably, the operators $\hat{W}_p$ commute with each other and with the Hamiltonian (1.1). This greatly simplifies our problem since the total Hilbert space $L$ can now be divided into sectors $L\{W_1, \ldots, W_N\}$ for different sets of eigenvalues $\{W_1, \ldots, W_N\}$, with $N$ being the total number of plaquettes. This can be written as follows:

$$L = \bigoplus_{\{W_1, \ldots, W_N\}} L\{W_1, \ldots, W_N\}$$

It is quite clear from equation (1.2) that $\hat{W}_p^2 = 1$, the eigenvalues of every operator $\hat{W}_p$ is then either $+1$ or $-1$. Thereby a sector can be seen as a particular choice of $W_p = \pm 1$ for each plaquette $p$. For reasons that will become clear later, these $\mathbb{Z}_2$ operators will be called flux operators. If $W_p = +1$ the plaquette $p$ is said to be flux-free, if $W_p = -1$ the plaquette has a flux.

As a consequence of the above remarks, the Hamiltonian $\hat{H}_K$ can be brought into block-diagonal form, the problem being now to diagonalize it within each subspace $L\{W_1, \ldots, W_N\}$. In a system with $N$ unit cells with periodic boundary conditions, there are $2N$ sites for $N$ different plaquettes, the full Hilbert space $L$ has dimension $2^{2N}$ but only $2^N$ different flux sectors exist. Hence, each sector has still an exponentially large size of $2^{2N}/2^N = 2^N$ and the solution remains a challenging problem.

1.2.2 Majorana representation

As shown by Kitaev, the Hamiltonian $\hat{H}_K$ projected on each sector may be mapped onto non-interacting fractionalized quasi-particles. In particular, the fractionalization is performed in terms of Majorana fermions. Introduced by Ettore Majorana in 1937 [11], Majorana fermions are particles that are their own anti-particles, unlike for example electrons. This means in the operator language that we have the following relations: $\hat{\gamma} = \hat{\gamma}^\dagger$ and $\hat{\gamma}^2 = 1$.

One direct consequence of these unusual properties is that the occupation number is not well-defined, hence labelling $\hat{\gamma}$ as a particle is somewhat misleading. One way to get around this issue is to view $\hat{\gamma}$ rather like a fractionalized zero-mode comprising half of a regular fermion [12]. A pair of Majorana fermions $\hat{\gamma}_1$ and $\hat{\gamma}_2$ must always be combined to form an ordinary (complex) fermion

$$\hat{f} = \frac{1}{2}(\hat{\gamma}_1 + i\hat{\gamma}_2)$$
Chapter 1. Kitaev’s honeycomb lattice model

and it is then possible to construct a vacuum state which is annihilated by all standard destruction operators. Despite obeying the usual anti-commutation relations, the fermion $f$ remains non-trivial in two critical aspects. First, $c_1$ and $c_2$ can localize arbitrarily far apart from one another, consequently $f$ encodes highly non-local entanglement. Second, one can empty or fill the non-local state described by $\hat{f}$ with no energy cost, this results in a ground state degeneracy.

The Majorana fractionalization consists in representing each spin with four Majorana fermions $\hat{b}^x_i$, $\hat{b}^y_i$, $\hat{b}^z_i$ and $\hat{c}_i$ as depicted in figure 1.2. The former operators $\hat{\sigma}^\alpha_i$ are mapped onto new spin operators $\tilde{\sigma}^\alpha_i$ defined as follows:

$$\tilde{\sigma}^x_i = i\hat{b}^x_i \hat{c}_i, \quad \tilde{\sigma}^y_i = i\hat{b}^y_i \hat{c}_i, \quad \tilde{\sigma}^z_i = i\hat{b}^z_i \hat{c}_i$$

(1.5)

Given the following anti-commutation relations $\{\hat{b}^\alpha_i, \hat{b}^\beta_j\} = 2\delta_{ij}\delta_{\alpha\beta}$ and $\{\hat{c}_i, \hat{c}_j\} = 2\delta_{ij}$, the spin commutation relations for $\tilde{\sigma}^\alpha_i$ are correctly reproduced.

The Majorana representation of spins $\frac{1}{2}$ is in fact overcomplete. Indeed, each Majorana fermion has a notional Hilbert space dimension $\sqrt{2}$, as a result the four Majorana fermions per spin have a total Hilbert space dimension of $(\sqrt{2})^4 = 4$ doubling the size of the Hilbert space per spin. The direct consequence is that the possible states can be grouped into physical and unphysical states and it is necessary to project out the latter in order to get only the relevant physical informations. For an extensive discussion on the physical many-body states in the Majorana description, we refer to [2] and a very complete analysis in [13].

![Figure 1.2](image.png)

Figure 1.2: Representation of spins in terms of four Majorana fermions. Picture taken from [2].

1.2.3 Application to the model

Let us now apply the Majorana representation to the Kitaev Hamiltonian $\hat{H}_K$ (1.1). The coupling terms become $\tilde{\sigma}^\alpha_i \tilde{\sigma}^\alpha_j = (i\hat{b}^\alpha_i \hat{c}_i)(i\hat{b}^\alpha_j \hat{c}_j) = -i(i\hat{b}^\alpha_i \hat{b}^\alpha_j)\hat{c}_i\hat{c}_j$. We
1.2. Exact solution

define the Hermitian operator \( \hat{u}_{ij} \equiv i \tilde{u}_{ij}^{\alpha} \tilde{b}_{ij}^{\alpha} \) (depicted in figure 1.2), the Hamiltonian then reads:

\[
\hat{H}_u = i \sum_{\langle ij \rangle} J^\alpha_{ij} \hat{u}_{ij} \hat{c}_i \hat{c}_j
\]  

(1.6)

where the summation is over all nearest-neighbour bonds. We follow the convention that \( i \) (resp. \( j \)) is located on sublattice \( A \) (resp. \( B \)). Remarkably, the operators \( \hat{u}_{ij} \) commute with each other and with the Hamiltonian \( \hat{H}_u \), thus the \( \{ u_{ij} \} \) are constants of motion with \( u_{ij} = \pm 1 \). Similarly to (1.3) we may write \( \tilde{L} = \bigoplus_u \tilde{\hat{L}}_u \), where \( u \) stands for the collection of all \( u_{ij} \). The restriction of Hamiltonian (1.6) to the subspace \( \tilde{\hat{L}}_u \) is obtained by “removing the hats”, i.e., replacing operators by numbers. This procedure results in the Hamiltonian

\[
\hat{H}_u = \frac{i}{2} \left( \hat{c}_A^T \hat{c}_B \right) \begin{pmatrix} 0 & M^T \\ -M & 0 \end{pmatrix} \left( \begin{pmatrix} \hat{c}_A \\ \hat{c}_B \end{pmatrix} \right)
\]  

(1.7)

which corresponds to free fermions. Here \( M \) is an \( N \times N \) matrix with elements \( M_{ij} = J^\alpha_{ij} u_{ij} \), and \( \hat{c}_A(B) \) is a vector of \( N \) Majorana operators on the \( A(B) \) sublattice.

It is possible to express in the Majorana representation the flux operators \( \hat{W}_{p} \) defined in section 1.2.1. A direct calculation shows that it can be expressed in terms of the bond operators \( \hat{u}_{ij} \), as follows

\[
\hat{W}_p = \hat{u}_{12} \hat{u}_{23} \hat{u}_{34} \hat{u}_{45} \hat{u}_{56} \hat{u}_{61}
\]  

(1.8)

The same holds also for their eigenvalues: \( W_p = u_{12} u_{23} u_{34} u_{45} u_{56} u_{61} \). It is quite clear from the latter relation that there are many distinct sets \( \{ u_{ij} \} \) that give rise to the same flux sector \( \{ W_1, \ldots, W_N \} \). For example flipping all bonds emanating from the same site does not change the flux sector. In particular transforming the coupling of all bonds \( J^\alpha \rightarrow -J^\alpha \) is equivalent to changing each bond variable form \( u_{ij} \rightarrow -u_{ij} \), which does not affect the flux sector. The redundancy of the emergent \( \mathbb{Z}_2 \) gauge fields \( \hat{u}_{ij} \) is a consequence of the transformation to Majorana operators which has increased the size of the Hilbert space. Hence the problem takes the form of non-interacting Majorana fermions coupled to a static \( \mathbb{Z}_2 \) gauge field, where the physical properties of the system depend on the flux sector only. A detailed analysis the Hilbert space dimensions, the gauge degrees of freedom and the different flux sectors is given in [13].

The eigenmodes of \( \hat{H}_u \) can be found via a singular-value decomposition of \( M \), giving \( M = U S V^T \) where \( U \) and \( V \) are \( N \times N \) orthogonal matrices, and \( S \) is an \( N \times N \) diagonal matrix containing the non-negative singular values of \( M \). We define new Majorana operators according to

\[
(\hat{c}'_{A,1}, \cdots, \hat{c}'_{A,N}) = (\hat{c}_{A,1}, \cdots, \hat{c}_{A,N}) U
\]  

(1.9)

\[
(\hat{c}'_{B,1}, \cdots, \hat{c}'_{B,N}) = (\hat{c}_{B,1}, \cdots, \hat{c}_{B,N}) V
\]  

(1.10)
For a given set of \( \{u_{ij}\} \), the Hamiltonian can be decomposed into the form

\[
\hat{H}_u = \frac{i}{2} \left( \hat{c}_A^T \hat{c}_B^T \right) \left( \begin{array}{cc} U & 0 \\ 0 & V \end{array} \right) \left( \begin{array}{cc} 0 & S^T \\ -S & 0 \end{array} \right) \left( \begin{array}{cc} U^T & 0 \\ 0 & V^T \end{array} \right) \left( \begin{array}{c} \hat{c}_A \\ \hat{c}_B \end{array} \right)
\]

where \( \epsilon_m \geq 0 \) are the singular values of \( M \). It is convenient to combine the Majorana operators \( \hat{c}_{A,m}^\prime \) and \( \hat{c}_{B,m}^\prime \) into canonical fermions \( \hat{a}_m^\prime = \frac{1}{2} (\hat{c}_{A,m}^\prime + i \hat{c}_{B,m}^\prime) \). This eventually gives

\[
\hat{H}_u = \sum_{m=1}^{N} \epsilon_m \hat{a}_{A,m}^\dagger \hat{a}_{B,m}^\prime - 1
\]

with the ground-state energy \( E_0 = -\sum_{m=1}^{N} \epsilon_m \). Eigenstates of the Hamiltonian (1.6) can thus be understood as direct product of "gauge" (\( u \)) and "matter" (\( a \)) degrees of freedom.

**Analogy to graphene.** An alternative way of finding the ground state and excitation spectrum is by solving the tight-binding model of complex fermions \( \hat{d} \) on the hexagonal lattice with nearest-neighbor hopping, i.e. the tight-binding model for graphene. Diagonalizing the Hamiltonian \( \hat{H}_{tb} \)

\[
\hat{H}_{tb} = \frac{i}{2} \left( \hat{d}_A^T \hat{d}_B^T \right) \left( \begin{array}{cc} 0 & M \\ M^T & 0 \end{array} \right) \left( \begin{array}{c} \hat{d}_A \\ \hat{d}_B \end{array} \right)
\]

gives a particle-hole-symmetric spectrum with eigenvalues \( \pm S_m \). In this case, we find eigenmodes of energy \( \epsilon_m \), while excitations in the Majorana model have energy \( 2\epsilon_m \). Moreover the tight-binding model exhibits hole like excitations, thus its ground state is not fermion free. Nevertheless, one can obtain the singular values \( S_m \) by taking only one set of eigenvalues with \( S_m \geq 0 \). The transformation matrix \( \hat{X} \) that diagonalizes the tight-binding Hamiltonian is related to the matrices of the singular-value decomposition \( U, V \) by

\[
\hat{X} = \left( \begin{array}{cc} U & -U \\ V & V \end{array} \right)
\]

The Kitaev model, however, is a spin Hamiltonian and the similarity to graphene is lost if we would for example consider the Kitaev model in a magnetic field [2].

**1.3 Properties of the ground state**

A theorem of Lieb [14] guarantees that the ground state of the Kitaev model in the thermodynamic limit, is located in the flux-free sector. We choose the
1.3. Properties of the ground state

flux free state by setting all \( u_{ij} = +1 \). In this sector, the system is translation-invariant and the excitation spectrum of the hopping Hamiltonian \( \hat{H}_{u=1} \) can be found using a Fourier transformation.

The general procedure is as follows. Let us represent the site index \( j \) as \((s, \lambda)\), where \( s \) refers to a unit cell, and \( \lambda \) to a position type inside the cell (we choose the unit cell as shown in figure 1.1). The Hamiltonian becomes \( \hat{H}_u = (i/2) \sum_{s,\lambda,t,\mu} A_{s\lambda,t\mu} c_{s\lambda} c_{t\mu} \), where \( A_{s\lambda,t\mu} \) actually depends on \( \lambda, \mu, \) and \( t - s \). Then we pass to the momentum representation:

\[
\hat{H}_u = \frac{1}{2} \sum_{q,\lambda,\mu} i\tilde{A}_{\lambda\mu}(q)a_{-q,\lambda}a_{q,\mu}
\]

\[
\tilde{A}_{\lambda\mu}(q) = \sum_{t} e^{i(q \cdot r_t)} A_{0\lambda,t\mu}
\]

\[
a_{q,\lambda} = \frac{1}{\sqrt{2N}} \sum_{s} e^{-i(q \cdot r_s)} c_{s\lambda}
\]

The spectrum \( \epsilon(q) \) is given by the eigenvalues of the matrix \( i\tilde{A}_{\lambda\mu}(q) \). We call it "double spectrum" because of the relation \( \epsilon(q) = -\epsilon(-q) \). The "single spectrum" can be obtained by taking only the positive eigenvalues. For the Hamiltonian (1.6), we have \( A_{ij} = J^{\alpha}_{ij} u_{ij} \), giving the following results:

\[
i\tilde{A}(q) = \begin{pmatrix} 0 & if(q) \\ -if(q)^* & 0 \end{pmatrix}
\]

\[
f(q) = 2(J^x e^{i(q \cdot n_1)} + J^y e^{i(q \cdot n_2)} + J^z)
\]

\[
\epsilon(q) = \pm |f(q)|
\]

with the lattice vectors \( n_1 = \left( \frac{1}{2}, \frac{\sqrt{3}}{2} \right) \) and \( n_2 = \left( -\frac{1}{2}, \frac{\sqrt{3}}{2} \right) \) given in figure 1.1.

After applying an appropriate Bogoliubov transformation [13], we map the operators \( a_{q,\lambda} \) onto new fermionic operators \( a'_{q,\lambda} \) such that the Hamiltonian is diagonalized and we arrive at:

\[
\hat{H}_{u=1} = \sum_{q} \epsilon(q)(a'^\dagger_q a'_q - \frac{1}{2})
\]

The ground state is a state without fermions, \( a'_q |0\rangle = 0 \) and the ground state energy is \( \epsilon_0 = -\frac{1}{2} \sum_q \epsilon(q) \).

The excitation spectrum \( \epsilon(q) \) of fermionic matter excitations \( a'^\dagger_q |M_0\rangle \) is gapless when the equation \( J^x e^{i(q \cdot n_1)} + J^y e^{i(q \cdot n_2)} + J^z = 0 \) has solutions. That is if and only if \( |J^x|, |J^y|, |J^z| \) satisfy the triangle inequalities:

\[
|J^x| \leq |J^x| + |J^y|, \quad |J^y| \leq |J^x| + |J^z|, \quad |J^z| \leq |J^y| + |J^z|
\]

Therefore the gapless and gapped phases (named \( B \)) extend according to the figure 1.3a. At the isotropic point \( J^x = J^y = J^z \), the dispersion resembles
that of graphene with fermions hopping on the honeycomb lattice, see figure 1.3b. In the gapless phase, there are two Dirac points at \( K = \left( \frac{2\pi}{\sqrt{3}}, \frac{2\pi}{3} \right) \) and \( K' = \left( \frac{2\pi}{\sqrt{3}}, -\frac{2\pi}{3} \right) \) (for \( J_x = J_y = J_z \)) with a linear energy spectrum \( \epsilon(q) \propto |q| \) in their close vicinity, see figure 1.3b. Once the exchange constants become anisotropic the Dirac points start to move in the Brillouin zone until they merge and annihilate, such that for \( |J^z| > |J^x| + |J^y| \) (and permutations) the spectrum becomes gapped.

(a) Phase diagram of the model [2] \hspace{1cm} (b) Spectrum at the isotropic point [9]

Figure 1.3: On the left side, the triangle is the section of the positive octant \((J_x, J_y, J_z \geq 0)\) by the plane \( J_x + J_y + J_z = 1 \). The diagrams for the other octants are similar. On the right side, the spectrum \( E(q) \) of the matter fermions in the ground state flux sector is shown in the first Brillouin zone at the isotropic point \( J_x = J_y = J_z \). The two Dirac cones lead to a linearly vanishing density of states at low energies.
Chapter 2

Impurities in the Kitaev model

The presence of defects - like vacancies, impurities or lattice distortions - is inherent in any real material. It is therefore important to have a theoretical understanding to be able to explain experimental observations. Indeed, these defects can fundamentally change the physical behaviour of the whole system and even sometimes lead to new phases. One striking example of that is the metal-insulator transition induced by disorder [15].

Besides, introducing impurities and looking at the response can provide knowledge about the system and can help distinguish between possible phases. In particular, impurities are a privileged tool to study spin liquids. Due to the absence of any symmetry breaking order in these systems, we rely essentially on indirect measurements to detect characteristic spin liquid behaviour. In chapter 4 we will study the local responses that can be experimentally measured.

This chapter is organized in two parts: after having developed an appropriate scattering theory, we apply it to detect the existence of bound states.

2.1 Scattering theory

A scattering problem can generally be stated as follows: an incident particle in a state $|\psi_0\rangle$ is scattered by a potential $\hat{V}$ resulting in a scattered state $|\psi_s\rangle$. The incident state $|\psi_0\rangle$ is assumed to be an eigenstate of the unperturbed Hamiltonian $\hat{H}_0$. The aim of a scattering theory is to solve the eigenvalue problem of the full perturbed Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$, in other words:

$$ (\hat{H}_0 + \hat{V})|\psi\rangle = E|\psi\rangle \quad (2.1) $$

where the eigenvalues $E$ and the eigenstates $|\psi\rangle$ are to be found.
In the following, we describe first the type of impurity we will consider in this thesis, we present next the $T$-matrix formalism.

### 2.1.1 The bond impurity

We will only consider in this thesis the case of an impurity consisting of a flipped bond, that is the following change of interaction $J_{ij}^{\alpha} \rightarrow -J_{ij}^{\alpha}$ between two sites $i$ and $j$. In the framework of the Majorana Hamiltonian (1.6), this impurity takes the form: $\hat{V}_{\text{flip}} = -2iJ_{ij}^{\alpha} \hat{u}_{ij} \hat{c}_i \hat{c}_j$.

It is however possible to view this perturbation from a different angle, in particular the transformation $\hat{u}_{ij} \rightarrow -\hat{u}_{ij}$ leads exactly to the same perturbation. Thus, as we can see from equation 1.8, the impurity has in fact a direct impact on the fluxes $\hat{W}_p$. We know from the previous chapter that the ground state of the unperturbed system is located in the flux-free sector where $W_p = +1$ for all plaquettes. Changing the sign of $\hat{u}_{ij}$ leads to the change of sign of the two flux operators in which $\hat{u}_{ij}$ appears, consequently a pair of fluxes is inserted through the plaquettes either side of the flipped bond $\langle ij \rangle$ as shown in the figure 2.1.

![Figure 2.1: A bond flip (green bond) leads to the insertion of a pair of $\mathbb{Z}_2$ gauge fluxes. Picture taken from [9].](image)

As a result, the bond flip can rather be viewed as the insertion of a flux pair and the ground state of the perturbed system is then located in the two-flux sector. As we mentioned earlier, different choices of gauge can give the same sector. Zschocke discussed in section 4.7 in [13] some subtleties of the model, namely that the projection of states on the physical space depends in some ways on the chosen gauge.

The type of boundary conditions has also a great impact on the response of the system. We develop this subject in appendix A and explain why we used periodic boundary conditions based on different criteria related to symmetries, gauge invariance and numerical efficiency.
2.1.2 The Lippmann-Schwinger equation

The Lippmann-Schwinger equation [16] relates an eigenstate $|\psi\rangle$ of the perturbed Hamiltonian $\hat{H}$ to an eigenstate $|\phi_0\rangle$ of the unperturbed Hamiltonian $\hat{H}_0$ in the following way:

$$|\psi\rangle = |\psi_0\rangle + \hat{G}_0(\omega)V|\psi\rangle$$

(2.2)

where we used a compact notation by introducing the unperturbed Green’s function defined as

$$\hat{G}_0(\omega) = \lim_{\epsilon \to 0} (\omega - \hat{H}_0 + i\epsilon)^{-1}$$

(2.3)

The term $i\epsilon$ is added to enforce causality by making sure that the scattered state $|\psi\rangle - |\psi_0\rangle$ has no incoming probability current associated with it [17]. Equation (2.2) is implicit and can be solved in fact recursively, let us rearrange it as follows:

$$|\psi\rangle = |\psi_0\rangle + \hat{G}_0(V + \hat{V}\hat{G}_0\hat{V} + \hat{V}\hat{G}_0\hat{V}\hat{G}_0\hat{V} + \ldots)|\psi_0\rangle$$

(2.4)

The term in parenthesis is defined as the $\hat{T}$-matrix, its expression can be simplified given that the infinite sum is a geometric series up to factor $\hat{V}$. We have:

$$\hat{T} = \hat{V} + \hat{V}\hat{G}_0\hat{V} + \hat{V}\hat{G}_0\hat{V}\hat{G}_0\hat{V} + \ldots$$

(2.5)

$$\hat{T} = \hat{V}(1 - \hat{G}_0\hat{V})^{-1}$$

(2.6)

The $\hat{T}$ matrix can be seen as the sum of scattering events of all orders for a single impurity. The important aspect of these calculations is that we can now write the eigenstate $|\psi\rangle$ of $\hat{H}$ in terms of unperturbed variables:

$$|\psi\rangle = |\psi_0\rangle + \hat{G}_0(\omega)V\hat{T}|\psi_0\rangle$$

(2.7)

The perturbed Green’s function $\hat{G}$ can be obtained similarly [13]:

$$\hat{G} = \hat{G}_0 + \hat{G}_0\hat{T}\hat{G}_0$$

(2.8)

2.1.3 Adapting the $T$-matrix method

We have to adapt the $T$-matrix formalism developed above in the case of a two-site scatterer, since the flipped bond links two lattice sites. To do so, we need to consider a potential having the following matrix form:

$$\hat{V}(r_0) = \begin{pmatrix} 0 & V^{AB} \\ V^{BA} & 0 \end{pmatrix}$$

(2.9)

where $V_{AB} = V_{BA} \equiv v$ is the potential for a particle hopping from the $A$ site to the $B$ site of the unit cell located at $r_0$ or vice versa. Similarly, the Green’s functions introduced earlier should also take this matrix form, we have:

$$\hat{G}_0(r, r') = \begin{pmatrix} G_{0}^{AA}(r, r') & G_{0}^{AB}(r, r') \\ G_{0}^{BA}(r, r') & G_{0}^{BB}(r, r') \end{pmatrix}$$

(2.10)

Due to sublattice symmetries, we have: $G_{0}^{AA}(r, r) = G_{0}^{BB}(r, r) \equiv g_0$ and $G_{0}^{AB}(r, r) = G_{0}^{BA}(r, r) \equiv g_1$. Note that $g_0$ and $g_1$ do not depend anymore on the position $r$, ...
but still on $\omega$. We deduce the expression of the perturbed Green’s function $\hat{G}$ from equation (2.8):

$$\hat{G}(r, r') = \hat{G}_0(r, r') + \hat{G}_0(r, r_0)T\hat{G}_0(r_0, r')$$

(2.11)

### 2.1.4 Expressions for the Green’s functions

As we will see later on, the density of states requires the computation of on-site Green’s functions, let us then obtain the expressions of $\hat{g}_0$ and $\hat{g}_1$.

It is important to keep in mind that this method is valid as long as particle-hole symmetry holds, which means that we need to consider the equivalent tight-binding model (1.15). The Lehmann representation of the Green’s function is given by [13]

$$g_0(\omega) = \hat{G}_0^{AA}(r, r, \omega) = \sum_{m}^{2N} \frac{\langle A^b_0 | \hat{d}_{A,r} | m \rangle \langle m | \hat{d}_{A,r}^\dagger | A^b_0 \rangle}{\omega - \epsilon_m}$$

(2.12)

$$= \sum_{m}^{2N} \frac{X_{im}X_{im}}{\omega - \epsilon_m}$$

(2.13)

$$= \sum_{m}^{N} \left[ \frac{1}{2} \frac{U_{im}V_{jm}}{\omega - \epsilon_m} + \frac{1}{2} \frac{U_{im}V_{jm}}{\omega + \epsilon_m} \right]$$

(2.14)

where we took into account the fact that the eigenenergies come in pairs $\pm \epsilon_m$. Here $|m\rangle$ are the eigenstates and $i(j)$ is the lattice index of the $A(B)$ site of unit cell $r$ and $|A^b_0\rangle$ the ground state of $H_{tb}$. Similarly we find:

$$\hat{G}_0^{BB}(r, r, \omega) = \sum_{m}^{N} \left[ \frac{1}{2} \frac{V_{jm}V_{jm}}{\omega - \epsilon_m} + \frac{1}{2} \frac{V_{jm}V_{jm}}{\omega + \epsilon_m} \right]$$

(2.15)

$$g_1(\omega) = \hat{G}_0^{AB}(r, r, \omega) = \sum_{m}^{N} \left[ \frac{1}{2} \frac{U_{im}V_{jm}}{\omega - \epsilon_m} - \frac{1}{2} \frac{U_{im}V_{jm}}{\omega + \epsilon_m} \right]$$

(2.16)

For the later analysis it will be necessary to evaluate the density of states using the Majorana Hamiltonian, which has weights at energies $\omega \geq 0$ only. To calculate this quantity, we again use the Lehmann representation

$$\tilde{G}_0^{AA}(r, r, \omega) = \sum_{m}^{2N} \frac{\langle A_0 | \hat{a}_{r} | m \rangle \langle m | \hat{a}_{r}^\dagger | A_0 \rangle}{\omega - 2\epsilon_m}$$

(2.17)

where $|A_0\rangle$ is the ground state and $|m\rangle$ are now states of the Majorana Hamiltonian with eigenenergies $2\epsilon_m$. Using the transformation outlined in section 1.2.3,
2.2. Detecting the bound states

These Green's functions are thus found to be

\[ \tilde{G}_0^{AA}(r, r, \omega) = N \sum_m U^*_{im} U_{im} \frac{\omega - 2\epsilon_m}{\omega - 2\epsilon_m} \] (2.18)

\[ \tilde{G}_0^{BB}(r, r, \omega) = N \sum_m V^*_{jm} V_{jm} \frac{\omega - 2\epsilon_m}{\omega - 2\epsilon_m} \] (2.19)

\[ \tilde{G}_0^{AB}(r, r, \omega) = N \sum_m U^*_{im} V_{jm} \frac{\omega - 2\epsilon_m}{\omega - 2\epsilon_m} \] (2.20)

It demonstrates that for positive energies the Green's functions of the Majorana Kitaev model and the equivalent tight binding model are closely related but differ by a factor of two in weight and energy eigenvalues. This allows us to perform the $T$-matrix calculation for the equivalent tight binding model in order to obtain the density of states of the Majorana model.

2.2 Detecting the bound states

One goal of this chapter is to detect the possible bound states arising from the insertion of the impurity. One way to achieve this is to look directly at the density of states (DOS) of the perturbed system. Fortunately enough, there exists a rather simple relation between the local density of states (LDOS) and the local Green's functions:

\[ \rho_{A,B}(r, \omega) = -\frac{1}{\pi} \lim_{\epsilon \to 0} \text{Im} \tilde{G}_{AA, BB}(r, r, \omega + i\epsilon) \] (2.21)

For finite size systems, as we can see from our previous derivations (equations (2.8-2.14-2.16), the DOS takes the form of a sum of delta peaks located right at the eigenenergies. In the thermodynamic limit, close energy contributions can form a continuum but isolated states remain present as sharp peak contributions. We are specifically looking for bound states, i.e. localized states. This can be achieved knowing that in-gap states are exponentially localized [18]. Therefore, these in-gap states are signaled by persistent sharp contributions in the LDOS.

2.2.1 Necessary and sufficient conditions for bound states

It is easy to see from equation (2.8) that a singularity in the LDOS can only occur if the $T$ matrix itself has a singularity. Since $\hat{T} = \hat{V}(1 - \hat{\tilde{G}}_0 \hat{\tilde{V}})^{-1}$, the singularities arise when the matrix $1 - \hat{\tilde{G}}_0 \hat{\tilde{V}}$ is not invertible. Consequently, the equation giving the bound states energies $\omega$ is

\[ \det(\hat{I} - \hat{\tilde{G}}_0(\omega) \hat{\tilde{V}}) = 0 = (1 - g_1(\omega)v)^2 - (g_0(\omega)v)^2 \] (2.22)
This is equivalent to:

\[
\frac{1}{v} = g_1(\omega) \pm g_0(\omega) \tag{2.23}
\]

Let us analyse this equation. It is clear from equations (2.14) and (2.16) that we have \( g_1(\omega) = g_1(-\omega) \) and \( g_0(\omega) = -g_0(-\omega) \). This implies that for a solution \( \omega_0 \) of \( \frac{1}{v} = g_1(\omega) + g_0(\omega) \), then \(-\omega_0\) is a solution of \( \frac{1}{v} = g_1(\omega) - g_0(\omega) \). Therefore, every bound state energy comes by pair, and this is in fact consistent with the particle-hole symmetry of the tight-binding Hamiltonian 1.15.

The procedure is then the following: we solve the ”+” equation of (2.23) in \( \mathbb{R} \) and every solution gives another solution with opposite energy. Finally, to obtain the results for the Majorana Hamiltonian, we only keep the positive energies.

### 2.2.2 Numerical results

As mentioned earlier, we want to observe in-gap bound states. To do so, we must be located in the gapped phase of the Kitaev and thus choose the exchange constants \( J_x, J_y, J_z \) accordingly (see equation (1.24) and figure 1.3a). For simplicity, we will consider the following coupling constants:

\[
J_z = \beta, \quad J_x = J_y = \frac{1-\beta}{2} \quad \text{with} \quad J_x + J_y + J_z = 1 \tag{2.24}
\]

For \( \beta \in [\frac{1}{2}, 1] \) the spectrum of \( \hat{H}_{tb} \) acquires a gap between the two symmetric bands. The gap width can be derived from analytical calculations in this case and is equal to \( -\omega_{\text{gap}}, \omega_{\text{gap}} \) with \( \omega_{\text{gap}} = 2(2\beta - 1) \). By definition (see equations (2.14) and (2.16)), the functions \( g_0 \) and \( g_1 \) are continuous in this energy gap. In the following we will plot them only in this interval.

Since our perturbation is either the flip of \( J_z \)-bond or the inequivalent flip of \( J_{x,y} \)-bond, the potential is either \( v = -2J_z \) or \( v = -2J_{x,y} \) respectively. We define the function:

\[
f_{BS}(\omega) = -2J_i[g_0(\omega) + g_1(\omega)] \tag{2.25}
\]

If we have \( f_{BS}(\omega_0) = 1 \) then \( \omega_0 \) is a solution of the bound state equation (2.23), which means there exists a bound state with energy \( \omega_0 \). The function \( f_{BS} \) is plotted in figure 2.2 for different \( i = x, y, z \) and different \( \beta \)s.

The conclusion of the figure 2.2 is clear: the functions \( f_{BS} \) never touch the line \( y = 1 \), therefore there is no solution of the bound state equation, there are no bound states arising in the gapped phase of the Kitaev model.
2.2. Detecting the bound states

Figure 2.2: Function $f_{BS}$ in the case of a $J_z = \beta$ bond flip impurity (solid lines) and in the case of a $J_x = (1 - \beta)/2$ bond flip impurity (dashed lines) for different $\beta$. $f_{BS}$ is plotted only in the gap. The simulations have been performed with a lattice containing $N = 900$ sites.
Chapter 3

Kekulé distortion in the Kitaev model

The conclusion of the previous part was clear: there are no in-gap bound states arising from a bond flip in the original Kitaev model. The goal of the next chapters is to find a variant of the Kitaev model such that (1) its energy spectrum is gapped and (2) in-gap bound states arise when a bond impurity is inserted.

The question of opening a bandgap has already been asked in the context of graphene and received a number of different answers. Semenoff and Haldane showed successively in the 1980s that a bandgap could be opened by breaking inversion symmetry [19] or time reversal symmetry [20]. Other mechanisms have been discovered recently namely that mechanical strain applied on the lattice can also open significant energy gaps in graphene’s electronic spectrum [21]. Using this idea, a strained Kitaev model has been studied and revealed a number of remarkable features among them a gap opening, the realization of Landau levels for Majorana fermions and a mechanism of probe-induced bound-state formation [6].

Chamon, Hou, Ryu and Mudry studied a third approach which would break neither time-reversal symmetry nor the conservation of electronic charge [22, 23, 24]: they consider bond-density waves. In particular, we will study in this thesis a Kekulé-type of lattice distortion.

This chapter is organized in the following way: we present first the Kekulé distortion and we discuss some of its properties, then we study the energy spectrum as a function of the distortion strength and we provide a physical interpretation of the results.
3.1 The Kekulé distortion

The lattice distortion we will study in this thesis is inspired by the structure of benzene discovered by August Kekulé shown in figure 3.1b. The coupling interactions are modulated throughout the honeycomb lattice according to the pattern shown in figure 3.1a, thereby the bonds are split into two groups of bonds, \( h \)-bonds (for "hexagons") and \( i \)-bonds (for "inter-hexagons").

\[
\begin{align*}
J_{ij}^\alpha &= J^\alpha \text{ for } h \text{ bonds} \\
J_{ij}^\alpha &= \kappa J^\alpha \text{ for } i \text{ bonds}
\end{align*}
\]

Figure 3.1: (a) Two types of bonds are introduced into the Kekulé-distorted lattice: \( h \)-bonds (solid lines) and \( i \)-bonds (dashed lines). (b) This modulation is inspired by the Kekulé structure of benzene with alternating double and single carbon bonds.

The coupling constants are modulated in the following way:

\[
\begin{align*}
J_{ij}^\alpha &= J^\alpha \text{ for } h \text{ bonds} \\
J_{ij}^\alpha &= \kappa J^\alpha \text{ for } i \text{ bonds}
\end{align*}
\]

We will mainly focus on the isotropic case \( J^x = J^y = J^z = J \). The last section of this chapter will briefly tackle the anisotropic case.

3.1.1 Analogy to the Peierls distortion

It is possible to interpret the Kekulé distortion as the two-dimensional analogue of the Peierls distortion in one-dimensional systems. Indeed, at low temperatures many of monovalent one-dimensional crystals undergo a transition from metallic to insulating behavior. This phenomenon can be explained as follows: the atoms in the lattice rearrange slightly, moving from an equally-spaced crystal to one in which the spacing alternates, that is, the atoms form pairs as shown in figure 3.2.
3.1. The Kekulé distortion

Consequently the period of the crystal is doubled and the Brillouin zone is twice smaller. The band structure is deformed and a gap opens up around the Fermi energy, as a result the ground state energy in the "dimerized" configuration is lower than in the equally-spaced lattice [25].

\[
\begin{array}{c}
\bullet \bullet \bullet \bullet \bullet \bullet \\
\bullet \bullet \bullet \bullet \bullet \bullet \\
\end{array}
\]

Figure 3.2: Peierls’ distortion of one-dimensional periodic lattice.

The Kekulé $\sqrt{3} \times \sqrt{3}$ superstructure can be seen as a triangular Bravais lattice with a basis of 6 atoms per unit cell as shown in figure 3.3a. As a result, the number of energy bands is tripled and the Brillouin zone is reduced by a factor $\sqrt{3}$ (solid hexagon in figure 3.3b) compared to the Brillouin zone of an homogeneous isotropic honeycomb lattice (dotted hexagon in figure 3.3b). In particular, the positions of $K$ and $K'$ in momentum space are given by $K = \left( \frac{2\pi}{3\sqrt{3}a}, \frac{2\pi}{9a} \right)$ and $K' = \left( \frac{2\pi}{3\sqrt{3}a}, -\frac{2\pi}{9a} \right)$ where $a$ is the distance between two nearest-neighbour sites.

(a) Unit cell of the distorted lattice

(b) Brillouin zones

Figure 3.3: (a) Unit cells of the distorted lattice are represented in grey, the basis vectors of the Bravais lattice are $e_1, e_2$. We show also a specific numbering of the sites and the interaction couplings of the bonds. (b) First Brillouin zone of the Kekulé distorted lattice with reciprocal vectors $b_1, b_2$ showing the symmetry points $\Gamma, M, K$ and $K'$. The Brillouin zone of the isotropic lattice is shown in dotted lines with the corresponding symmetry points $M_{iso}, K_{iso}$ and $K'_{iso}$. 
As we have done in section 1.3 of chapter 1, due to translation invariance with the basis vectors $e_1, e_2$, the excitation spectrum can be obtained performing a Fourier transformation. The unit cell containing now 6 sites, we get the following 6×6-matrix:

\[
\tilde{A}(\mathbf{q}, \kappa) = J \begin{bmatrix}
0 & 0 & 0 & \kappa e^{-i\mathbf{q} \cdot \mathbf{e}_2} & 1 & 1 \\
0 & 0 & 0 & 1 & \kappa e^{i\mathbf{q} \cdot (\mathbf{e}_2 - \mathbf{e}_1)} & 1 \\
0 & 0 & 0 & \kappa e^{i\mathbf{k} \cdot \mathbf{e}_2} & 1 & 1 \\
1 & \kappa e^{i\mathbf{k} \cdot (\mathbf{e}_1 - \mathbf{e}_2)} & 1 & 0 & 0 & 0 \\
1 & 1 & \kappa e^{-i\mathbf{k} \cdot \mathbf{e}_1} & 0 & 0 & 0
\end{bmatrix}
\] (3.3)

where we used the numbering given in figure 3.3a.

The energy spectrum is obtained diagonalizing the matrix $\tilde{A}(\mathbf{q}, \kappa)$ and the positive eigenvalues $\epsilon(\mathbf{q})$ correspond to the energy bands of the Majorana fermions. The two following sections present and interpret the band structure for $\kappa < 1$ first and for $\kappa > 1$ in a second phase.

### 3.2 Energy spectrum for $\kappa < 1$

Let us analyse now the band structure and the energy spectrum as a function of the distortion $\kappa \in [0, 1]$.

(a) Energy spectrum
3.2. Energy spectrum for $\kappa < 1$

(b) Band structure for $\kappa = 0.25$ (left), $\kappa = 0.5$ (middle), $\kappa = 0.75$ (right)

Figure 3.4: (a) Energy bands $\epsilon(q)$ represented along the cut $M \Gamma K M$ in the Brillouin zone for different values of $\kappa$. (b) Energy spectrum plotted as a function of the distortion strength $\kappa \in [0, 1]$. The shaded region indicates the bands in the flux-free sector. The dots represent the numerical energy spectrum $\epsilon_n$ (see equation 1.14) computed from a lattice of $N = 2025$ unit cells.

The figures 3.4b-3.4b reveal the existence of two distinct gapped phases: for $0 < \kappa < \frac{3}{4}$, one of the three bands is separated from the others resulting in the formation of an inter-band gap, for $\frac{3}{4} < \kappa < 1$ the three bands touch and a low-energy gap remains. Let us discuss in more details these results.

### 3.2.1 Behaviour close to $\kappa = 1$

There is no modulation at $\kappa = 1$ therefore we recover the gapless spectrum of the isotropic Kitaev model extending continuously from $\epsilon = 0$ to $\epsilon = 6J$.

As we saw previously for the Kitaev model discussed in chapter 1, inhomogeneities of the couplings could shift the Dirac cones in the Brillouin zone, in the end leading to their annihilation by merging [2]. Here, the figure 3.4a shows that the spectrum becomes gapped as soon as $\kappa \neq 1$ and the formation of a gap has a different origin. As mentioned earlier, the size of the Brillouin zone is decreased by the distortion and it is necessary to fold the points $K_{iso}$, $K'_{iso}$ and $M_{iso}$ (see figure 3.3b) into the new smaller Brillouin zone. The Dirac points $K_{iso}$ and $K'_{iso}$ get folded to the $\Gamma$ point after some translation by the reciprocal vectors $b_i$, hence they are coupled to each other and a gap opens up.

The gap opens up linearly at $\Gamma$ with an energy $\epsilon_{\Gamma} = (\kappa - 1)J$ (obtained via symbolic computations).

### 3.2.2 Behaviour close to $\kappa = 0$

At $\kappa = 0$, the lattice consists of separated hexagons made of $h$ bonds. As we can see from figure 3.4a, the spectrum is discrete and hence the bands are flat. This can be easily deduced from the form of the matrix $\tilde{A}(q, \kappa)$ (equation 3.3) since setting $\kappa = 0$ remove the momentum dependence. Physically speaking, this is a
Chapter 3. Kekulé distortion in the Kitaev model

consequence of the fact that the hexagons are independent of each other and of finite size.

The energy eigenvalues can be obtained analytically. One hexagon can be considered as a one-dimensional chain containing 6 fermions with periodic boundary conditions. As in section 1.2.3 of chapter 1, the model is made out of complex standard fermions, we will in the end truncate the spectrum and keep only the positive energies doubled to get the Majorana spectrum. The hopping Hamiltonian of this hexagonal ring reads:

\[ \hat{H}_\Box = J \sum_{n=0}^{5} (\hat{d}_n^\dagger \hat{d}_{n+1} + \hat{d}_{n+1}^\dagger \hat{d}_n) \]  

(3.4)

with the operators \( \hat{d}_n^\dagger \) (\( \hat{d}_n \)) creating (destroying) a fermion at site \( i \). Let us decompose an eigenstate \( |\Psi\rangle \) of \( \hat{H}_\Box \) in the basis \( |i\rangle \) which is the state with one fermion occupying the site \( i \), the other sites remaining empty. We write \( |\Psi\rangle = \sum_{i=0}^{5} c_i |i\rangle \) with some complex numbers \( c_i \). Denoting \( E \) the energy of \( |\Psi\rangle \), we have:

\[ \hat{H}_\Box |\Psi\rangle = E |\Psi\rangle \]  

(3.5)

\[ J \sum_{n=0}^{5} (\hat{d}_n^\dagger \hat{d}_{n+1} + \hat{d}_{n+1}^\dagger \hat{d}_n) \sum_{i=0}^{5} c_i |i\rangle = E \sum_{i=0}^{5} c_i |i\rangle \]  

(3.6)

\[ J \sum_{i=0}^{5} (\hat{d}_{i-1}^\dagger \hat{d}_i + \hat{d}_{i+1}^\dagger \hat{d}_i + c_i |i\rangle = E \sum_{i=0}^{5} c_i |i\rangle \]  

(3.7)

We apply the bra \( \langle j | \) on the above equation, this yields:

\[ \langle j | \sum_{i=0}^{5} (\hat{d}_{i-1}^\dagger \hat{d}_i + \hat{d}_{i+1}^\dagger \hat{d}_i) c_i |i\rangle = \langle j | E \sum_{i=0}^{5} c_i |i\rangle \]  

(3.8)

\[ J (c_{j+1} + c_{j-1}) = E c_j \]  

(3.9)

We choose the ansatz \( c_j = A e^{i(j\theta)} \). The periodic boundary conditions are taken into account with the relation: \( c_0 = c_6 \) which implies that \( \theta = \frac{2\pi m}{6} \) with \( m = 0, \ldots, 5 \). Since the state \( |\Psi\rangle \) should be normalized to unity, we deduce the value of \( A = \frac{1}{\sqrt{6}} \). From equation 3.9, the eigenstates and eigenenergies are obtained as a function of \( m \):

\[ |\Psi^{(m)}\rangle = \frac{1}{\sqrt{6}} \sum_{j=0}^{5} e^{i \frac{2\pi jm}{6}} |j\rangle \]  

(3.10)

\[ E^{(m)} = 2J \cos \left( \frac{2\pi m}{6} \right) \]  

(3.11)

The positive values of \( E^{(m)} \) occur for \( m = 0, 1, 5 \). After doubling these energies, we get the Majorana spectrum at \( \kappa = 0 \) which consists of \( \epsilon = 2J \) with a double degeneracy and \( \epsilon = 4J \) as one can see in figure 3.4a.
3.2.3 Behaviour in the bulk

The figure 3.3b suggests that the band edges are reached at the symmetry points of the Brillouin zone. The lower energy band seems to reach its minimum at $\Gamma$ and its maximum at $M$, symbolic computations give the following expression $\epsilon = 2J \pm 2\kappa J$. As for the upper energy band, the edges are hit at $K$ (minimum) and at $\Gamma$ (maximum). Its highest energy value is $\epsilon = 4J + 2\kappa J$ and its lowest energy is $\epsilon = 2\sqrt{\alpha^2 - 2\alpha + 4}$. These results agree very well to the numerical points in figure 3.4a. These analytical expressions allowed to obtain that at $\kappa = \frac{3}{4}$ the inter-band gap closes up. The band structure (figure 3.4b) shows that this mid-gap is in fact indirect.

3.3 Energy spectrum for $\kappa > 1$

Let us analyse now the band structure and the energy spectrum as a function of the distortion $\kappa \in [1, +\infty]$.

The figure 3.5a displays the following features: first, a lower gap opens up as soon as $\kappa \neq 1$, this can be explained as before by the coupling of the two Dirac cones. For any $\kappa > 1$, the three bands touch each other and the band energy form a continuum. As $\kappa$ increases, the energy band gets narrower and becomes point-like at $\kappa = +\infty$ in units of $\kappa J$.

(a) Energy spectrum
(b) Band structure for $\kappa = \frac{4}{3}$ (left), $\kappa = 2$ (middle) and $\kappa = 4$ (right)

Figure 3.5: (a) Energy bands $\epsilon(q)$ represented along the cut $M\Gamma KM$ in the Brillouin zone for different values of $\kappa$. (b) Energy spectrum plotted as a function of the distortion strength $\kappa \in [1, +\infty]$. Note that the horizontal axis is linear in $\kappa/(1 + \kappa)$ while the vertical axis is linear in $\kappa J$. The shaded region indicates the bands in the flux-free sector. The dots represent the numerical energy spectrum $\epsilon_n$ (see equation 1.14) computed from a lattice of $N = 2025$ unit cells.

### 3.3.1 Behaviour close to $\kappa = +\infty$

In the limit $\kappa \to +\infty$, the spectrum becomes point-like when scaled in units of $\kappa J$, however the figures 3.5b show that the bandwidth remains finite no matter how big is $\kappa$. This can be understood if we perform perturbation theory on the quantity $\frac{1}{\kappa}$ for the matrix $\tilde{A}(q)$:

$$
\frac{\tilde{A}}{\kappa J}(q) = \tilde{H}_\infty + \frac{1}{\kappa} \tilde{V}_\infty \quad \text{with} \quad \tilde{V}_\infty = \begin{bmatrix}
0 & 0 & 0 & 0 & 1 & 1 \\
0 & 0 & 1 & 0 & 1 \\
0 & 0 & 1 & 1 & 0 \\
0 & 1 & 1 & 0 & 0 \\
1 & 0 & 1 & 0 & 0 \\
1 & 1 & 0 & 0 & 0
\end{bmatrix}
$$

and

$$
\tilde{H}_\infty = \begin{bmatrix}
0 & 0 & 0 & e^{-i\mathbf{q} \cdot \mathbf{e}_2} & 0 & 0 \\
0 & 0 & 0 & 0 & e^{i\mathbf{q} \cdot (\mathbf{e}_2 - \mathbf{e}_1)} & 0 \\
0 & 0 & 0 & 0 & 0 & e^{i\mathbf{q} \cdot \mathbf{e}_1} \\
e^{i\mathbf{k} \cdot \mathbf{e}_2} & 0 & 0 & 0 & 0 \\
0 & e^{i\mathbf{k} \cdot (\mathbf{e}_1 - \mathbf{e}_2)} & 0 & 0 & 0 \\
0 & 0 & e^{-i\mathbf{k} \cdot \mathbf{e}_1} & 0 & 0
\end{bmatrix}
$$

The Hamiltonian $\tilde{H}_\infty$ has one positive eigenvalue $\epsilon = 1$ with a three-fold degeneracy. Therefore, applying degenerate perturbation theory, we obtain the following energy expansion:

$$
\epsilon_n(k) = 2\kappa J + f_n(k)J + o\left(\frac{1}{\kappa}\right)
$$
Due to the triple degeneracy, the energy is split into three bands \( f_n(k) \) with the following analytical expressions:

\[
\begin{align*}
  f_1(k) &= -2 \\
  f_{2,3}(k) &= 1 \pm \sqrt{1 + 4 \cos \left( \frac{3k_y a}{2} \right)^2 + 4 \cos \left( \frac{3\sqrt{3} k_x a}{2} \right) \cos \left( \frac{3k_y a}{2} \right)}
\end{align*}
\]  

The energy bands \( f_i(k) \) are plotted in figure 3.6a. The band structure is rich and displays a number of remarkable features like the existence a flat band, multiple degeneracies in particular with a quadratic-linear band touching at the \( K \) point for the bands \( f_{2,3}(k) \). In fact, these features are characteristic of a tight-binding model on a Kagome lattice (shown in figure 3.6b) and have been extensively discussed in [26, 27]. This relation becomes clear in the limit \( \kappa \to \infty \) when the lattice consists of a Kagome \( i \)-bond lattice.

![Figure 3.6](image)

Figure 3.6: (a) Energy bands \( f_n(k) \) along the cut \( M\Gamma KM \) in the Brillouin zone. (b) Kagome lattice.

### 3.4 Distortion and anisotropic couplings

So far we considered a Kekulé distortion with isotropic couplings \( J \). Let us now consider the anisotropic case \( J^x \neq J^y \neq J^z \) and focus on whether the spectrum is gapless or gapped. This results in the phase diagram below where we have analytically computed the phase boundaries.

In the isotropic case, the Kekulé modulation couples the two Dirac points which are gapped out, hence the spectrum is gapped for any \( \kappa \neq 1 \). In contrast, the anisotropic Kitaev model at \( \kappa = 1 \) displays Dirac cones which are shifted in momentum space, an extended gapless phase remains for \( \kappa \neq 1 \) - this applies to \( J^z/J^x,y < 1 \) and \( 1 < J^z/J^x,y < 2 \) [2]. Remarkably, the gapless phases extend all the way to \( \kappa \to 0 \) and \( \kappa \to +\infty \). The phase diagram cannot be understood
Figure 3.7: Phase diagram of the Kekulé-modulated Kitaev model as function of the distortion strength $\kappa$ and anisotropy $J_z/J_{x,y}$

only reasoning in terms of folding of bands, otherwise the gapless phase would not extend higher than $J_z/J_{x,y} > 2$. 
Chapter 4

Impurities in the Kekulé-distorted Kitaev model

The previous chapter showed that a Kekulé distortion applied on the isotropic Kitaev model induces the opening of multiple energy gaps in the spectrum. It is time to see whether in-gap bound states can arise when the system is perturbed by local impurities.

This has been studied in fact in different forms in the context of graphene. Chamon showed that midgap polaronic states could emerge in carbon nanotubes modulated by a Kekulé pattern [22]. Hou, Chamon and Mudry discovered that fractionally charged excitations could exist in a Kekulé version of graphene appearing as topological zero-modes [23]. More recently, Rachel, Fritz and Vojta studied a strained Kitaev model and uncovered the realization of Landau levels for Majorana fermions and a mechanism of probe-induced bound-state formation [6].

This chapter is organized as follows: we study the response of a Kekulé-distorted Kitaev model perturbed by a bond impurity for different distortion strengths $\kappa$, next we compute and interpret the spin correlations of the system which can be experimentally measured.

4.1 Response to the impurities

We study in the following the effect of a bond impurity on the spectrum of the Kekulé-distorted Kitaev system. Before going further, it is important to distinguish the two possible cases: the flip of either a $h$-bond or a $i$-bond. These types of bond flip correspond to two types of flux pairs.
Therefore we define an $h$-impurity as an $h$-bond flip or equivalently as the insertion of a pair of flux through a ”blue” plaquette (made up of $h$ bonds) and a ”green” plaquette (made up of $h$ bonds and $i$ bonds with equal proportion) as shown in figure 4.1. Likewise, we define an $i$-impurity as an $i$-bond flip or equivalently as the insertion a pair of flux through two ”green” plaquettes. We will opportune switch from one representation to the other in the rest of this chapter.

(a) An $h$-impurity

(b) An $i$-impurity

Figure 4.1: (a) An $h$-impurity is inserted, the bond flip is a $h$-bond colored in red, the fluxes are inserted through two different types of plaquettes indicated in blue and green shaded areas. (b) An $i$-impurity is inserted, the bond flip is a $i$-bond colored in red, the fluxes are inserted through two ”green” plaquettes.

4.1.1 Numerical results

Let us study the response of the Kekulé-distorted Kitaev system to perturbation. The figure below superposes the spectrum of a system perturbed by successively a single $h$-impurity or a single $i$-impurity.
4.1. Response to the impurities

Figure 4.2: Superposition of the energy spectrum of a Kekulé-distorted Kitaev system perturbed by either a single $h$-impurity or a single $i$-impurity plotted as a function of $\kappa$. The shaded region indicates the bands in the flux-free sector. The energy levels lying outside of the shaded region have been highlighted, namely we used circles for the spectrum corresponding to the $h$-impurity, and cross for the spectrum corresponding to the $i$-impurity. The dots represent the numerical energy spectrum $\epsilon_n$ computed from a lattice of $N = 2025$ unit cells.

The figure 4.2 displays a number of striking features. First, when a single $h$-impurity is inserted, the figure shows the emergence of in-gap energy levels for any distortion $\kappa$. More precisely, for $\kappa < 1$, two almost degenerate states - the energy difference cannot be seen on the figure - arise in the inter-band gap as long as the latter exists, that is in the range $[0, \frac{3}{4}]$. Another bound state arises in the lower gap close to zero energy and exist for any $\kappa \in [0, 1]$. For $\kappa > 1$, one bound state lies below the energy band and stays close the lower edge until merging with it as $\kappa$ goes to infinity.

Second, when a single $i$-impurity is inserted, no in-gap states are produced for $\kappa < 1$ but one energy level appears for $\kappa > 1$ in the lower gap and stay lower than the bound state produced by a $h$-impurity all the way to $\kappa = \infty$.

Finally, the perturbed spectrum for both type of impurities does not radically change from the unperturbed spectrum, apart from the appearance of a small number of new energy levels. This is clearly visible by the perfect overlap between the numerical energy levels represented by the dots and the unperturbed spectrum represented by the grey shaded area. Since the perturbation is carried by a two-site scatterer, its energy should scale as $\frac{1}{N}$ with $N$ being the number of
Chapter 4. Impurities in the Kekulé-disorted Kitaev model

unit cells in the system. Therefore, no energy band shift or opening are expected because they would involve perturbations of larger magnitude capable of shifting an infinite number of states.

Since an $h$-impurity consists of flipping a $J$-coupling and an $i$-impurity consists of flipping a $\kappa J$-coupling, we expect the effect of a $h$-impurity to be more important than the effect of a $i$-impurity for $\kappa < 1$, and conversely for $\kappa > 1$.

4.1.2 Analysis of the bound states energies

It is possible to obtain analytically the energy eigenvalues of the perturbed system at $\kappa = 0$. In this situation, the interaction on $i$-bonds is turned off and it is clear that an $i$-impurity does not actually change the system - since $0 = -0$. Let us then focus on the $h$-impurity case. As we did in section 3.2.2 of the previous chapter, we can consider an associated hopping problem on a perturbed hexagon, comprising now one negative hopping coupling. Obtaining the eigenvalues of this ”perturbed” ring can be achieved in the same way as before. Keeping the same notations, we write an eigenstate of $\hat{H}_\circ$ as follows $|\Psi\rangle = \sum_{i=0}^{5} c_i |i\rangle$ where the complex numbers $c_i$ obey the following recurrence (equation (3.9)):

$$J(c_{j+1} + c_{j-1}) = E c_j$$

We choose again the same ansatz $c_j = Ae^{i(j\theta)}$. However, to take into account the negative hopping coupling, we choose antiperiodic boundary conditions i.e. $c_0 = -c_6$. This implies that $\theta = \frac{\pi}{6}(2m + 1)$ with $m = 0, \ldots, 5$. Inserting this expression in equation (3.9), the eigenenergies are obtained as a function of $m$:

$$E^{(m)} = 2J \cos \left( \frac{\pi}{6} (2m + 1) \right)$$

The positive values of $E^{(m)}$ are obtained for $m = 0, 1, 4, 5$. After doubling these energies, we get $\epsilon = 0$ (we removed one degeneracy) and $\epsilon = 2\sqrt{3}J$ with a two-fold degeneracy. Since there is only one single $h$-impurity inserted in the system, hence only one perturbed hexagon, the Majorana spectrum at $\kappa = 0$ consists of a superposition of the eigenvalues of unperturbed ($\epsilon = 2J$ and $\epsilon = 4J$) and perturbed ($\epsilon = 0$ and $\epsilon = 2\sqrt{3}J$) hexagons.

Quite remarkably for $\kappa < 1$, the isolated energy levels stay approximately at the same value for any $\kappa$ until merging with the bands at $\kappa = \frac{3}{4}$ for the mid states and $\kappa = 0$ for the lower state. This happens in some extent for $\kappa > 1$, the isolated energies are approximately linear in $\kappa J$ and merge with the bands at $\kappa = 1$ and $\kappa = +\infty$. This can be understood as a consequence of their isolation, indeed they are in some way decoupled from the energy bands.

This latter point can be understood more formally invoking the concept of adiabatic continuity introduced by Anderson [28]. The idea is that a strongly interacting system retains some of the properties of its non-interacting parent (obtained at $\kappa = 0$ in our case, consisting of a set of decoupled hexagons). With the interactions being slowly turned on (i.e. increasing $\kappa$), there is a continuous mapping of the excitations of an non-interacting system with that
4.1. Response to the impurities

of the interacting system. Thus the quantum numbers describing one excitation state are still valid even after the interactions are fully applied, provided no phase transition occurs. The absence of bound states with an $i$-impurity for $\kappa < 1$ can be explained by adiabatic continuity. There are no in-gap states in this case since there are no such states at $\kappa = 0$.

4.1.3 Wavefunctions of the in-gap states

So far we detected the appearance of isolated in-gap states. It has been pointed out in [18] that in-gap states must yield a bound state around the impurity. Let us show the wavefunctions for the different in-gap states found earlier. The wavefunction of an eigenmode $m$ is given by $w_{A,i}^m = U_{mi}$ and $w_{B,i}^m = V_{mi}$ with the $U$ and $V$ matrices coming from the singular value (1.7).

Figure 4.3: Wavefunctions of the bound states for $\kappa = 0.5$ with an $h$-impurity (a-b-c) and $\kappa = 2$ with an $h$-impurity (d) and an $i$-impurity (e). The red (blue) color indicates a positive (negative) weight on the site in question. The inserted pair of fluxes is indicated with the same color notations as in figure 4.1. We only show a truncated view centered on the impurity, the other sites have vanishing weights. We perform the calculations on a lattice with $N = 225$ unit cells.
The figure 4.3 shows as expected that all these in-gap states are localized around the impurity. These bound states can be classified according to their signature under reflection at the flipped bond. For $\kappa = 0.5$, the low-energy bound state (panel a) is even, whereas the two higher-energy states are odd (panel b) and even (panel c). For $\kappa = 2$, the $h$-impurity leads to an even bound state (panel d), whereas the $i$-impurity produces an odd bound state (panel e).

Moreover, the highest weights are located around the $h$-plaquette (colored in yellow) for $\kappa = 0.5$, whereas they are located around the $i$-plaquettes (colored in magenta) for $\kappa = 2$. This seems to suggest that these states localize on the plaquette having the strongest couplings between its sites.

4.2 Bound-state spectroscopy

So far, we have demonstrated the presence of bound states formed by matter Majorana fermions and $\mathbb{Z}_2$ gauge fluxes (or pairs thereof). Such bound states are directly visible in spectroscopic probes, and we show this by determining the dynamic spin structure factor for the Kekulé-distorted Kitaev model.

4.2.1 Dynamic spin structure factor

Dynamical spin correlations in the Kitaev model have been explicitly calculated in [4]. Let us summarize the main steps below, we refer the reader to [29, 4] for details. Consider the zero-temperature spin correlation function

$$S_{ij}^{\alpha\beta}(t) = \langle 0|\hat{\sigma}_i^\alpha(t)\hat{\sigma}_j^\beta(0)|0\rangle$$  \hspace{1cm} (4.2)

where $|0\rangle$ is the many-body ground state. Given that the fluxes are constants of motion, the correlator can be calculated by decomposing the ground state $|0\rangle$ as a direct product of the ground states in the gauge and matter sector.

Specifically, the application of a $\hat{\sigma}_i^\alpha$ operator changes the two flux variables which involve the $\alpha$ bond emanating from site $i$. For the flux-free sector, this leads to $u_{(ij)\alpha} = -1$. As a result, if $\langle ij \rangle_\alpha$ is a $h$-bond ($i$-bond), the effect a $\hat{\sigma}_i^\alpha$ operator on the ground state is equivalent to the insertion of an $h$-impurity ($i$-impurity).

This leads to the dynamical rearrangement of matter fermions in the modified gauge field. The spin correlator can therefore be expressed purely in terms of matter fermions in the ground-state flux sector, subject to a perturbation $\hat{V}_\alpha = -2iJ^n\hat{c}_i\hat{c}_j$ [30, 4]. The spin correlators can be expressed in terms of Majorana fermions and yield the following Lehmann representation at zero temperature [29, 4], here written separately for the on-site correlator

$$S_{ii}^{\alpha\beta}(\omega) = 2\pi \sum_\lambda |\langle M_0|\hat{c}_i|\lambda\rangle|^2 \delta(\omega - (E_\lambda - E_0))\delta_{\alpha\beta}$$  \hspace{1cm} (4.3)
and the off-site correlators

\[ S_{ij}^{\alpha\beta}(\omega) = 2\pi F_{ij}^\alpha \sum_\lambda \langle M_0|\hat{c}_i|\lambda\rangle\langle\lambda|\hat{c}_j|M_0\rangle\delta(\omega - (E_\lambda - E_0))\delta_{\alpha\beta}\delta_{(ij),\alpha} \]  

(4.4)

where \( \delta_{(ij),\alpha} \) is non-zero only if \( i \) and \( j \) are nearest neighbors connected by an \( \alpha \) bond, i.e., \( S_{ij} \) vanishes beyond nearest neighbors. In both cases \( |M_0\rangle \) is the matter-fermion ground state of \( \hat{H}_0 \) in the ground-state flux sector, assumed to be flux-free, and \( \sum_\lambda \) runs over all matter-fermion states in the two-flux sector, i.e., the eigenstates of \( \hat{H}_0 + \hat{V}_\alpha \). \( E_0 \) and \( E_\lambda \) are the corresponding many-body energies. The prefactor \( F_{ij}^\alpha = \{-1, i, -i\} \) depending on the spin component. In order to evaluate the matrix elements \( \langle M_0|\hat{c}_i|\lambda\rangle \), involving eigenstates of both \( \hat{H}_0 + \hat{V}_\alpha \) and \( \hat{H}_0 \), we follow the procedure outlined in [29, 4].

We determine the spin structure factor in the single-mode approximation which has been shown to yield highly accurate results throughout the phase diagram of the standard Kitaev model [4, 29].

Below we will show results for the dynamic structure factor at momentum \( \mathbf{q} \),

\[ S^{\alpha\alpha}(\mathbf{q},\omega) = \frac{1}{N} \sum_{ij} e^{i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)} S_{ij}^{\alpha\beta}(\omega) \]  

(4.5)

4.2.2 Numerical results

Numerical results for the zero-temperature dynamic spin structure factor are shown in figure 4.4. Two striking features are apparent:

First, the bound states discussed in previous section show up as \( \delta \) peaks (represented by red bars) in \( S(\mathbf{q},\omega) \) at any fixed \( \mathbf{q} \). Interestingly, the peaks occur on top of a continuum contribution. This can be understood as follows: the momentum-dependent structure factor involves contributions both from flipped \( h \)- and flipped \( i \)-bonds. The corresponding flux gaps are different, such that the two contributions come with continua which are shifted by a different flux "offset", this can be clearly seen in figures 4.4c and 4.4d showing the \( h \)-impurity contribution (black) and the \( i \)-impurity contribution. Indeed, the gaps in the structure factor are smaller than the Majorana band gaps in figures 3.4a and 3.5a. The bound states in the two-flux sector occur in the corresponding spectral gap.

Second, there is little momentum dependence in the spin response. In particular, the bound-state peaks are non-dispersive which is a simple consequence of the fluxes (and hence the bound states) being localized. However, the weight of the bound-state peaks is momentum-dependent, as shown in figure 4.5.

Unfortunately, a subtlety in the choice of gauge - evoked in appendix A - leads to a number of issues on the numerical side. We were not able to produce consistent figures in the case \( \kappa > 1 \).
Figure 4.4: Total dynamic spin structure factor for the Kekulé-distorted Kitaev model as function of energy and momentum for coupling ratios (a)-(c) $\kappa = 0.3$, (b)-(d) $\kappa = 0.5$ as would be measured in inelastic neutron scattering and electron spin resonance. Top: $S(q,\omega)$ on a logarithmic color scale as a function of $\omega$ along the cut $M\Gamma KM$ through the Brillouin zone. Bottom: dynamic susceptibility $S_i(q=0,\omega)$. The red contributions correspond to an $i$-impurity, the black contributions to an $h$-impurity.

4.3 Discussion and outlook

The use of distortion has fulfilled our expectations: it is possible to open multiple energy gaps with a width that can be controlled by the distortion strength. This allowed us to search for bound states after applying perturbation to the system. The conclusion is then clear: in-gap localized states effectively arise when a pair of flux is inserted. This impurity corresponds in fact to the effect of a probe when spin correlations measurement are performed. We finally provided a theoretical estimation of the total dynamic structure factor and interpreted it highlighting the measurable contribution of the bound states.
Figure 4.5: Bound states weight as a function of momentum through the cut $MTKM$ in the Brillouin zone. The weights are expressed in percentage with respect to the total integrated weight $S(q, \omega)$. 
Appendix A

Boundary conditions

This appendix is devoted to the different possible choices of boundary conditions. In our work, we chose to use periodic boundary conditions. This decision is explained in the following.

A.1 Different types of boundary conditions

Using periodic boundary conditions (PBC) consists in identifying sites located at opposite sides of the lattice boundaries. The considered system is then transformed into a torus. This transformation can be performed with a twist $M$ as defined in the figure below: Contrary to PBC, there is no fold procedure for open boundary conditions (OBC).

Note that we could also consider a mix of both type of boundary conditions: the cylindrical boundary conditions. This is performed using PBC on only one side of the lattice and letting the other side open. We did not consider this option in the thesis.

A.2 Translation invariance and disorder

The main advantage of periodic boundary conditions is that the system then respects translation invariance. The respect of translation invariance becomes an issue however when it comes to studying systems that breaks this symmetry. In particular, this is the situation when local impurities are introduced. The local impurity is then infinitely duplicated, which is of course something that we want to avoid. To fix this, we need to manipulate systems big enough so that we can safely neglect the multiple occurrences of the impurity.

Using open boundary conditions is a more suitable choice when disorder is introduced. Contrary to PBC, it has clearly the advantage of not duplicating the inserted impurity.
Figure A.1: Honeycomb lattice with basis vectors $e_{1,2}$ and an illustration of the periodic boundary conditions, characterized by the cluster size $L_{1,2}$ and the twist parameter $M$. The figure corresponds to $L_1 = L_2 = 3$ and $M = 2$. Figure taken from [29].

A.3 Numerical efficiency and other subtleties

The calculations of spin correlators in chapter 4 is a striking example of the difference in numerical efficiency between the two possibilities. Indeed, for PBC every site is equivalent to the others, hence it is only needed to compute one spin correlator $S_{ij}$ per equivalent bond $\langle ij \rangle$. In contrast, with OPC every site is inequivalent, therefore $N$ spin correlators $S_{ij}$ have to be calculated compared to at most 2 for PBC in our case.

In some cases, a certain type of periodic conditions is simply not applicable for particular systems. This the case for instance for the tri-axial strained lattice considered in [6].

The type of boundary conditions has also an influence on the projection process which allows to get the physically relevant states. We refer to [13] in which much details are given.
Bibliography


