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Edge States and Zero Modes in Quadratic Fermionic Models on a 1-D Lattice

Relatore:
Prof.ssa Elisa Ercolessi

Presentata da:
Chiara Agostinelli

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To my parents.

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Chiara Agostinelli

Abstract

In una formulazione rigorosa della teoria quantistica, la definizione della varietà Riemanniana spaziale su cui il sistema è vincolato gioca un ruolo fondamentale.
La presenza di un bordo sottolinea l'aspetto quantistico del sistema: l'imposizione di condizioni al contorno determina la discretizzazione degli autovalori del Laplaciano, come accade con condizioni note quali quelle periodiche, di Neumann o di Dirichlet. Tuttavia, non sono le uniche possibili. Qualsiasi condizione al bordo che garantisca l'autoaggiunzione dell' operatore Hamiltoniano è ammissibile. Tutte le possibili *boundary conditions* possono essere catalogate a partire dalla richiesta di conservazione del flusso al bordo della varietà.
Alcune possibili condizioni al contorno, permettono l'esistenza di stati legati al bordo, cioè autostati dell' Hamiltoniana con autovalori negativi, detti *edge states*.
Lo scopo di questa tesi quello di investigare gli effetti di bordo in sistemi unidimensionali implementati su un reticolo discreto, nella prospettiva di capire come simulare proprietà di *edge* in un reticolo ottico.
Il primo caso considerato è un sistema di elettroni liberi. La presenza di *edge states* è completamente determinata dai parametri di bordo del Laplaciano discreto. Al massimo due edge states emergono, e possono essere legati all' estremità destra o sinistra della catena a seconda delle condizioni al contorno. Anche il modo in cui decadono dal bordo al bulk è completamente determinato dalla scelta delle condizioni.
Ammettendo un' interazione quadratica tra siti primi vicini, un secondo tipo di stati emerge in relazione sia alle condizioni al contorno che ai parametri del bulk. Questi stati sono chiamati *zero modes*, in quanto esiste la possibilità che siano degeneri con lo stato fondamentale.
Per implementare le più generali condizioni al contorno, specialmente nel caso interagente, è necessario utilizzare un metodo generale per la diagonalizzazione, che estende la tecnica di Lieb-Shultz-Mattis per Hamiltoniane quadratiche a matrici complesse.

Contents

Introduction

Since the early days of the quantum theory, boundary effects arise and play a crucial role; quantum theories on a Riemannian manifold requires the self-adjointness and positivity of the negative Laplacian of the system. In a compact boundary-less real manifold both properties are fullfilled; when the manifold is endowed with a boundary, the Laplacian may fail to be positive.
For instance, if a superconducting system is confined in a domain M with boundary Ω, the boundary conditions of the electromagnetic fields are predetermined by physics: they are time-reversal and also parity invariant for adapted geometry and they lead to edge excitations, while the bulk energies have a large gap.
A similar phenomenon occurs for topological insulator where appropriate boundary conditions for the Dirac Hamiltonian lead to similar edge states and incompressible bulk. Furthermore, this kind of edge states appears in QCD models with chiral boundary conditions[3].
Out of a relativistic approach, the crucial point is that edge states are a direct manifestation of the effects of topology in fermionic many-body systems. A prominent example is the quantum Hall effect, where chiral edge states are responsible for basic phenomena such as quantized transport.
In order to investigate edge properties, quantum simulation plays a central role, providing the possibility of using well-controlled quantum system to simulate the behaviour of an another one, whose dynamics escapes standard theorethical or experimental approaches. Geometry and topology are making their appearance in quantum simulators, specifically in optical lattice with ultra-cold atoms.
For 1-D optical lattice, artificial topology, that reproduces particular boundary conditions, has been implemented inducing appropriate hoppings on the internal degrees of freedom, attaining effectively higher-dimensional dynamics; for instance, a 1-D PBC hopping hamiltonian can be realized in a 1-D open lattice of L sites, each endowed with M internal states where the periodic boundary conditions could be induced technically operating on the system [9].
The possibility of manipulate boundary conditions in a controlled way paves the way for an accurate investigation of edge properties.
For instance, spinless fermions on a two-chain ladder driven by pair tunneling, show

zero-energy exitations on the edges of the ladder represented by Majorana fermions, in complete analogy with a one-dimensional topological superconductor [10].
These are only few examples that connect edge physics of lattice field theories to other quantum specific problems and make clear the importance of studying physics of lattices.

First of all, it is necessary to understand mathematically and analitically how edge states arise in a quantum field theory supported on a lattice, namely the lattice theory, before being able to implement them in a quantum simulator.
This master degree thesis inserts itself in this contest, regarding edge properties of a 1-D lattice of spinless fermions interacting through a quadratic potential, that reminds to the one considered in superconductivity theories. The aim is to give analytic solutions for edge states considering arbritary boundary conditions, in such a way to construct a general theory.
The implementation of arbritary boundary parameters, first of all, makes the diagonalization of the Hamiltonian not so obvious.
Furthermore, it is necessary to understand how such parameters provide a self-adjoint extension of the Hamiltonian in the continuum limit, in such a way the simulation of the theory on the discrete lattice is reasonable.
In the idea of deeply comprehending the treatment of general boundary conditions, the first step is to analyze the simple case of free electrons, where the diagonalization of the Hamiltonian that describes the system is easy to carry on. This will be done in Chapter 2. The eigenvalue problem may admit two possible kinds of solutions: scattering state, which always exist, that are a superposition of plane waves in the bulk and edge states, whose eigenfunction is mainly localised at the boundary, decaying exponentially from the edges. Boundary conditions fix the quantisation of the momentum of the bulk scattering states as well as the rate of decaying of the edge states. At most two edge states can emerge; they may be both bounded at one boundary point or splitted between the two ends of the chain. Of course, for some boundary conditions their presence is excluded.
Given the guidelines through the free case, the process may be extended for interacting electrons. However, the diagonalization of the Hamiltonian in this case requires a general method to include boundary conditions.
Lieb-Shultz and Mattis[12] in 1961 found a general way to diagonalize a quadratic Hamiltonian with two-bodies interaction terms. Neverthless, they supposed this interaction represented by a real matrix, which is not true in the description of a superconducting system or in the presence of a magnetic field. In Chapter 3, we will describe the standard LSM techinque and we will propose an extension of it applicable to complex operators.
Equipped with this new method of diagonalization, the procedure followed for free fermions can be performed in the interacting case.
As we will describe in Chapter 4, the interaction makes possible the emerging of new states, called $Zero\ Modes$, whose existence is determined both by boundary and bulk parameters; they can reach the zero energy point becoming degenerate with the ground

state. Such a degeneracy could give rise to a quantum phase transition.
As in the free case, at most two edge states are permitted. Furthermore, particular boundary conditions admit the presence of edge states and zero modes simultaneously.
The steps outlined above allowed us to build a general theory to describe the spectrum of quadratic fermionic hamiltonians with the most general boundary condition on 1D lattices. It would be interesting to check whether our techniques can be extended to higher dimensional systems, which have a wide range of applications, from topological insulators to lattice gauge theories.

Chapter 1

Preliminary Concepts

1.1 A simple example

A quantum theory must be compatible with the fondamental principle of the preservation of probability. This is the basic idea for implementing boundary conditions. Let us see, in a simple way, what it means.

Consider a non-relativistic point-like particle, moving on an one-dimensional Riemannian manifold[1] $M = [0, L]$ with smooth boundary $\Gamma = \partial M = \{0, L\}$ described by a free Hamiltonian:

$$H = -\frac{1}{2m}\frac{d^2}{dx^2}$$

For suitably differentiable functions on $([0, L])$ we have

$$\langle \phi_1, H\phi_2 \rangle = -\frac{1}{2m}\int_0^L \phi_1^* \ddot{\phi}_2 dx$$

where $\dot{\phi} = \frac{d\phi}{dx}$.
Let us consider $m = 1$ for sake of semplicity; integrating by parts, we get

$$\langle \phi_1, H\phi_2 \rangle - \langle \phi_2, H\phi_1 \rangle = -\frac{1}{2}\int_0^L \frac{d}{dx}\left[\phi_1^*\dot{\phi}_2 - \dot{\phi}_1^*\phi_2\right] dx = \Sigma(\phi_1, \phi_2) \tag{1.1}$$

with

$$\begin{aligned} \Sigma(\phi_1, \phi_2) =& \phi_1^*\dot{\phi}_2(L) - \dot{\phi}_1^*\phi_2(L) - \phi_1^*\dot{\phi}_2(0) + \dot{\phi}_1^*\phi_2(0) = \\ =& \left[\left(\phi_1^*\dot{\phi}_2 - \dot{\phi}_1\phi_2^*\right)\cdot\hat{n}\right]_0^L \end{aligned} \tag{1.2}$$

[1] For higher dimensional manifolds, see [4]

where $\hat{n}$ is, as usually, the normal versor[2].
This last term is what obstructs the self-adjointness of H. It has a relevant physical interpretation. It measures the net flux of probability across the boundary.
If the operator H has to be self-adjoint this flux must be null: the incoming flux has to be equal to the outgoing one, because the evolution operator e^{iHt} in such a case is unitary and preserves probability. For higher dimensional systems, this is just a version of the Gauss theorem.
It follows that the classification of the different possible self-adjoint extensions will be easily derived from the cancellation conditions of the boundary term $\Sigma(\phi_1, \phi_2)$, which can be written as a quadratic form of $(\phi, \dot{\phi} \cdot \hat{n})$

$$\Sigma(\phi_1, \phi_2) = (\phi_1^*, \phi_2^*) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \dot{\phi}_1 \\ \dot{\phi}_2 \end{pmatrix}$$

Furthermore, as explained in Appendix A, a self-adjoint extension H is given if exists a unitary matrix $V : \mathcal{R}(H - i\mathbb{I}) \to \mathcal{R}(H + i\mathbb{I})$ such that

$$V := (H + i\mathbb{I})(H - i\mathbb{I})^{-1} \tag{1.3}$$

called the Cayley transform of the operator. So, if V exists, there is also a partial Cayley transform for the Hamiltonian operator H_E acting on smooth functions belonging to the Hilbert space at the boundary, namely $\mathcal{H}(\Gamma)$.
H_E acts on $\phi|_{0,L}$ giving, because of Stokes theorem,

$$H_E \begin{pmatrix} \phi(0) \\ \phi(L) \end{pmatrix} = \begin{pmatrix} -\dot{\phi}(0) \\ \dot{\phi}(L) \end{pmatrix}$$

Hence, a unitary matrix U must provide the Cayley transform for H_E, namely:

$$H_E = -i(\mathbb{I} + U)(\mathbb{I} - U)^{-1} \tag{1.4}$$

U is a 2x2 matrix, considering that in this one-dimensional example, boundaries are provided by the two edge points 0 and L.
It follows that

$$\begin{aligned} (\mathbb{I} - U) \begin{pmatrix} -\dot{\phi}(0) \\ \dot{\phi}(L) \end{pmatrix} &= -i(\mathbb{I} + U) \begin{pmatrix} \phi(0) \\ \phi(L) \end{pmatrix} \\ \Rightarrow \quad \begin{pmatrix} -\dot{\phi}(0) + i\phi(0) \\ \dot{\phi}(L) + i\phi(L) \end{pmatrix} &= U \begin{pmatrix} \dot{\phi}(0) - i\phi(0) \\ -\dot{\phi}(L) - i\phi(L) \end{pmatrix} \end{aligned} \tag{1.5}$$

[2]In a N-dimensional manifold M, it is a N-versor orthogonal to the N-1-dimensional hypersurface ∂M.

It means that for every unitary matrix there exists an extension of H_E[3].
Some specially interesting cases are the following:

(i) *Periodic Boundary Conditions*

$$\begin{aligned} \phi(L) &= e^{i\theta}\phi(0) \\ \dot{\phi}(L) &= e^{i\theta}\dot{\phi}(0) \end{aligned} \tag{1.6}$$

In this case, as we know, eigenfunctions of H are given by $\phi_k(x) = Ae^{ikx}$ with $k = \frac{2\pi}{L}n$, $n \in \mathbb{Z}$. The role played by boundary conditions is to discretize the values of k.

(ii) *Neumann Boundary Conditions*

$$\phi(L) = \phi(0) = 0 \tag{1.7}$$

In this situation, the eigenfunctions of H are $\phi_k(x) = A\sin kx$ with $k = \frac{2\pi}{L}n$, $n \in \mathbb{Z}$.

(iii) *Dirichlet Boundary Conditions*

$$\dot{\phi}(L) = \dot{\phi}(0) = 0 \tag{1.8}$$

For such boundary conditions, eigenfunctions of H are caught by $\phi_k(x) = A\sin kx$ with $k = \frac{2\pi}{L}n$, $n \in \mathbb{Z}$..

(iv) *Robin Boundary Conditions*

$$\begin{aligned} \dot{\phi}(0) &= \lambda_1\phi(0) \\ \dot{\phi}(L) &= \lambda_2\phi(L) \end{aligned} \tag{1.9}$$

where λ_1, $\lambda_2 \in \mathbb{R}$. In such a case, there is a bulk spectrum $E_k^2 = k^2$, with plane wave eigenfunctions; neverthless, even solutions that are bounded to the edge are allowed, with eigenfunctions of the type

$$\phi(x) = ae^{\alpha x} + be^{-\alpha x}$$

[3]It may happens that $(\mathbb{I} - U)$ is singular. It is possible to define the Cayley transform swapping the roles of $(\mathbb{I} - U)$ and $(\mathbb{I} + U)$. In such a case a problem of definition arises if $(\mathbb{I} + U)$ is singular. Then, if we denote the eigenspace associated to the eigenvalue -1 with W, the self-ajoint extension H_E is given by the projection of the Cayley transform on the orthogonal subspace of W:

$$H_E = -iP_{W^\perp}(\mathbb{I} + U)(\mathbb{I} - U)^{-1}$$

However, smooth eigenfunctions of U with eigenvalue -1 still could be solutions, with negative energy, envisaging the presence of edge states.

In order to illustrate this, let us consider, for instance, the limit $\lambda_2 \to \infty$. From (1.9), it follows that

$$\alpha(a-b) = \lambda_1(a+b)$$
$$ae^{\alpha L} + be^{-\alpha L} = 0$$

Obtaining a and b and substituting in $\phi(x)$, we have an eigenfunction corresponding to a negative energy $E^2 = -|\lambda|^2$, which decays exponentially from the left edge $x = 0$. This is the reason why edge states are associated to negative energy eigenfuntions.

For a massive Dirac Hamiltonian, negative eigenvalues are not a problem for quantum field theory; however, such edge states arise requiring the conservation of density current at the boundary. Such a situation is what describes the case of a topological insulator[3]. We are going to work in a 1-D lattice of electrons, which are initially free and then interacting through a particular potential, considering the most general bondary parameters that must provide the self-adjoint extensions of the Hamiltonian in the continuum limit. We will find how to rewrite the H_E in terms of these parameters and we will analyze for which parameters edge states are admissible.
First of all, let us make a step back, in order to really comprehend that edge states have many phisical applications. One of this is in quantum computation. The presence of Majorana edge states in a 1-D fermionic interacting lattice, that produce two different phases for the system, could provide a quantum computational device.

1.2 Kitaev Model: an example for Majorana Edge States

Certain one-dimensional finite Fermi Systems can be used as qubits since they are intrinsically immune to problems of decoherence. Precisely it is possible, according to A.Y. Kitaev [14] to recognize a qubit on a site that can be either empty or occupied by an electron, usually with spin up (in these models the spin degree of freedom is not condidered). Such sites are called *local fermionic modes*.
Thanks to the conservation of charge, classical errors are avoided by placing the fermionic sites far apart from each other. In order to resolve also quantum problems of decoherence, that emerge as different phase for different electronic configurations, the idea is to consider " Majorana sites". An isolated Majorana site is immune to any kind of error.[4]
In particular, each fermionic site is described by a pair of annihilation and creation

[4]A full description of this decoherence-free property is out of the scope of this thesis. It can be found in [14]

operators a_j, $a_j^\dagger$. One can formally define *Majorana operators*:

$$c_{2j-1} = a_j + a_j^\dagger \quad , \quad c_{2j} = \frac{a_j - a_j^\dagger}{i} \qquad (j = 1, 2, ...L) \tag{1.10}$$

which satisfy the relations

$$c_m = c_m^\dagger \quad , \quad c_l c_m + c_m c_l = 2\delta_{lm} \qquad (l, m = 1, 2, ...2L) \tag{1.11}$$

According to this definition, it is possible, at least mathematically, to split each local fermionic mode into two objects, called Majorana fermions. The non-trivial idea is that, theoretically, they can be paired up by interaction, so that only a few Majorana fermions remain unpaired and separated from each other. Let us consider a chain of $L >> 1$ sites; the electron dynamics is described by the following Hamiltonian:

$$H = \sum_{j=1}^{L} \left(-\omega \left(a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j \right) - \mu \left(a_j^\dagger a_j + \frac{1}{2} \right) + \Delta a_j a_{j+1} + \Delta^* a_{j+1}^\dagger a_j^\dagger \right) \tag{1.12}$$

where

- ω is the hopping amplitude;
- μ is the chemical potential;
- $\Delta = |\Delta| e^{i\theta}$ is the superconducting gap.

Let's define the Majorana operators, including the phase parameter θ in the transformation:

$$c_{2j-1} = e^{i\frac{\theta}{2}} a_j + e^{-i\frac{\theta}{2}} a_j^\dagger \quad , \quad c_{2j} = -ie^{i\frac{\theta}{2}} a_j + ie^{-i\frac{\theta}{2}} a_j^\dagger \quad (j = 1, 2, ...L) \tag{1.13}$$

In terms of these new operators, the Hamiltonian becomes

$$H = \frac{i}{2} \sum_{j=1}^{L} \left(-\mu c_{2j-1} c_{2j} + (\omega + |\Delta|) c_{2j} c_{2j+1} + (-\omega + |\Delta|) c_{2j-1} c_{2j+2} \right) \tag{1.14}$$

Let us analyze this system at arbitrary values of ω, μ, Δ. It is necessary to reduce the Hamiltonian to a canonical form

$$H = \sum_{k=1}^{L} \epsilon_k \left(\tilde{a}_k^\dagger \tilde{a}_k - \frac{1}{2} \right) \tag{1.15}$$

that in terms of Majorana operators will appear as

$$H = \frac{i}{2}\sum_{k=1}^{L} \epsilon_k b'_k b''_k \tag{1.16}$$

where

$$\tilde{a}_k = \frac{1}{2}\left(b'_k + ib''_k\right)$$
$$\tilde{a}_k^\dagger = \frac{1}{2}\left(b'_k - ib''_k\right)$$

The diagonalization of H, as we will see in a more particular way in the last Chapter, brings to the following eigenvalues for the fermionic Hamiltonian:

$$\epsilon_k = \pm\sqrt{(2\omega\cos k + \mu)^2 + 4|\Delta|^2 \sin k^2} \quad -\pi \leq k \leq \pi \tag{1.17}$$

When $|\Delta| = \omega$ and $\mu = 0$ the eigenvalues become

$$\epsilon_k = \pm 2\omega = \pm 2|\Delta| \tag{1.18}$$

They are completely indipendent from k. What physically happens can be read from the Hamiltonian

$$H = i\omega\sum_{j=1}^{L} c_{2j}c_{2j+1} = 2\omega\sum_{j=1}^{L}\left(\tilde{a}_j^\dagger\tilde{a}_j - \frac{1}{2}\right)$$

where

$$\tilde{a}_j = \frac{1}{2}\left(c_{2j} + ic_{2j+1}\right) \quad \tilde{a}_j = \frac{1}{2}\left(c_{2j} - ic_{2j+1}\right)$$

are the fermionic operators transformed in order to make the Hamiltonian diagonal. The ground state is two-fold degenerate, since there are two orthogonal states, where the Majorana operators at the edge remain unpaired. One state has even fermionic parity, while the other one has odd parity, so that they represent two phases.

Figure 1.1: Two types of pairing.

Chapter 2

The Free Electron Case

We are going to analyze the case of non-interacting spinless fermions in a one-dimensional manifold. As we have seen in the first chapter, all possible boundary conditions must preserve the self-adjointness of the Hamiltonian operator.
We are going to consider a system of electrons on a discrete lattice of L+1 sites, with lattice step $a = 1$. In this situation, we are working with a finite number of degrees of freedom. Hence, the Hamiltonian is simply given by a (L+1)×(L+1) matrix, for which no difference between the notions of self-adjoint and symmetric exists[1]; it means that implementing boundary conditions merely consists in allowing arbritary parameters at the edges of the chain.
However, when the limit $a \to 0$ is approached[2], the discrete Laplacian becomes continuous and boundary parameters must provide a unitary matrix as its Cayley transform at the edge.
In this way all consistent self-adjoint extensions of the Hamiltonian are given and it is possible to classify them depending on the solutions they provide.
Moreover, we will see precisely that some extensions admit the presence at the edge of states described by real functions, the so-called edge states.

2.1 Discrete Lattice

As we already know, the Laplacian in one dimension is given by $\nabla^2 = \frac{d^2}{dx^2}$; so that when we have an eigeinvalues problem such as

$$-\nabla^2\psi(x) = k^2\psi(x)$$

[1]For finite dimensional linear operator, there are not problems in the definition of the domain of the adjoint operator. See Appendix A.

[2]The limit $a \to 0$ does not coincide with the thermodynamic limit, because the density of sites does not remain costant.

eigenfunction are provided by plane waves $\phi_k(x) = Ae^{ikx} + Be^{-ikx}$, where A and B are determined by boundary conditions and orthonormality request; it is simple to verify that their eigenvalues are $E_k^2 = k^2$. Considering a discrete Laplacian, instead, we have a finite difference operator acting on each site j:

$$-\nabla^2\psi_j = \psi_{j+1} + \psi j - 1 - 2\psi_j = E_k^2\psi_j \tag{2.1}$$

with a dispersion relation given by $E_k^2 = \cos^2 k$ and eigenfunctions

$$\psi_j = Ae^{ik(aj)} + Be^{-ik(aj)} \tag{2.2}$$

where a is the lattice step. Representing (2.1) through a matrix formalism on a lattice of L+1 sites, for periodic boundary conditions we have

$$H\begin{pmatrix} \psi_0 \\ \psi_1 \\ . \\ . \\ \psi_{L-1} \\ \psi_L \end{pmatrix} = \begin{pmatrix} -2 & 1 & 0 & . & . & .1 \\ 1 & -2 & 1 & 0 & . & . \\ . & . & . & . & . & . \\ .. & . & . & . & . & . \\ . & . & 1 & -2 & 1 & . \\ 1 & . & . & . & 1 & -2 \end{pmatrix} \begin{pmatrix} \psi_0 \\ \psi_1 \\ . \\ . \\ \psi_{L-1} \\ \psi_L \end{pmatrix} \tag{2.3}$$

Hence, a general Hamiltonian, describing particles on a lattice, must still share the same "diagonal" structure, with each site related to the two nearest neighbours.
Including *arbritary* boundary parameters, the most general fermionic Hamiltonian for a chain of L+1 sites is, then, provided by:

$$H = \begin{pmatrix} \mu & -t & 0 & . & . & . & 0 & 0 & u_A \\ -t & h & -t & 0 & . & . & . & 0 & 0 \\ 0 & -t & h & -t & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ 0 & . & . & . & . & . & . & -t & 0 \\ 0 & 0 & . & . & . & 0 & -t & h & -t \\ u_A^* & 0 & 0 & . & . & . & 0 & -t & \nu \end{pmatrix} \tag{2.4}$$

which in second quantization formalism, can be written as follows

$$\begin{aligned} H = \sum_{i=1}^{L-1} \left[-t\left(\hat{c}_{i-1}^\dagger\hat{c}_i + \hat{c}_{i+1}^\dagger\hat{c}_i\right) + h\hat{c}_i^\dagger\hat{c}_i\right] - t\left(\hat{c}_1^\dagger\hat{c}_0 + \hat{c}_{L-1}^\dagger\hat{c}_L\right) + \\ + u_A\hat{c}_0^\dagger\hat{c}_L + u_A^*\hat{c}_L^\dagger\hat{c}_0 + \mu\hat{c}_0^\dagger\hat{c}_0 + \nu\hat{c}_L^\dagger\hat{c}_L \end{aligned} \tag{2.5}$$

Boundary conditions consist of arbitrary chemical potentials μ and ν respectively for $i = 0$ and $i = L$, and of the hopping coefficient u_A between them, which represents in some way the possibility of a current from one edge to the other.
Now, the eigenvalue problem is well posed if $E_k\phi_k = H\phi_k$.
We are dealing with a traslational invariant Hamiltonian, at least far from the boundaries; so let us take plane waves as ansatz of solutions, namely:

$$\phi_k = \sum_{j=0}^{L} \left[ae^{ikj} + be^{-ikj}\right] \hat{c}_j^\dagger|0\rangle \tag{2.6}$$

Let us consider first the action of our Hamiltonian inside the bulk:

$$H_{bulk} = \sum_{i=1}^{L-1} \left[-t\left(\hat{c}_{i-1}^\dagger\hat{c}_i + \hat{c}_{i+1}^\dagger\hat{c}_i\right) + h\hat{c}_i^\dagger\hat{c}_i\right] - t\left(\hat{c}_1^\dagger\hat{c}_0 + \hat{c}_{L-1}^\dagger\hat{c}_L\right)$$

Applying it on our ansatz of solution, we obtain

$$\begin{aligned} H_{bulk}\phi = \sum_{i=1}^{L-1}\sum_{j=1}^{L-1} \left[-t\left(\hat{c}_{i-1}^\dagger\hat{c}_i + \hat{c}_{i+1}^\dagger\hat{c}_i\right) + h\hat{c}_i^\dagger\hat{c}_i\right] \left[ae^{ikj} + be^{-ikj}\right] \hat{c}_j^\dagger|0\rangle + \\ \sum_{i=1}^{L-1} \left[-t\left(\hat{c}_{i-1}^\dagger\hat{c}_i + \hat{c}_{i+1}^\dagger\hat{c}_i\right) + h\hat{c}_i^\dagger\hat{c}_i\right] [a+b]\, \hat{c}_0^\dagger|0\rangle + \\ \sum_{i=1}^{L-1} \left[-t\left(\hat{c}_{i-1}^\dagger\hat{c}_i + \hat{c}_{i+1}^\dagger\hat{c}_i\right) + h\hat{c}_i^\dagger\hat{c}_i\right] \left[ae^{ikL} + be^{-ikL}\right] \hat{c}_L^\dagger|0\rangle + \\ - t\left(\hat{c}_1^\dagger\hat{c}_0 + \hat{c}_{L-1}^\dagger\hat{c}_L\right) \sum_{j=0}^{L} \left[ae^{ikj} + be^{-ikj}\right] \hat{c}_j^\dagger|0\rangle \end{aligned}$$

that can be easily evaluated by using the fermionic anticommutation relations.

$$\hat{c}_\alpha^\dagger\hat{c}_\beta\hat{c}_\gamma^\dagger = \delta_{\gamma\beta}\hat{c}_\alpha^\dagger$$

The action on the bulk turns out to be

$$\begin{aligned} H_{bulk}\phi = \sum_{j=1}^{L-1} \left[ae^{ikj} + be^{-ikj}\right] \left[-t\left(\hat{c}_{j-1}^\dagger|0\rangle + \hat{c}_{j+1}^\dagger|0\rangle\right) + h\hat{c}_j^\dagger|0\rangle\right] + \\ - t\,[a+b]\,\hat{c}_1^\dagger|0\rangle - t\left[ae^{ikL} + be^{-ikL}\right] \hat{c}_{L-1}^\dagger|0\rangle \end{aligned}$$

We can manipulate this expression in order to get:

$$\begin{aligned} H_{bulk}\phi_k = \left[- t\left(e^{ik}+e^{-ik}\right)+h\right]\sum_{j=1}^{L-1}\left[ae^{ikj}+be^{-ikj}\right]\hat{c}_j^\dagger|0\rangle + \\ - t\left[ae^{ik}+be^{-ik}\right]\hat{c}_0^\dagger|0\rangle - t\left[ae^{ik(L-1)}+be^{-ik(L-1)}\right]\hat{c}_L^\dagger|0\rangle \end{aligned} \tag{2.7}$$

Now, let us consider the part of the Hamiltonian which operates at the edge, namely:

$$H_{edge} = u_A\hat{c}_0^\dagger\hat{c}_L + u_A^*\hat{c}_L^\dagger\hat{c}_0 + \mu\hat{c}_0^\dagger\hat{c}_0 + \nu\hat{c}_L^\dagger\hat{c}_L$$

It is easy to see that

$$H_{edge}\phi_k = \left[ae^{ikL}+be^{-ikL}\right]\left[u_A\hat{c}_0^\dagger|0\rangle + \nu\hat{c}_L^\dagger|0\rangle\right] + [a+b]\left[u_A^*\hat{c}_L^\dagger|0\rangle + \mu\hat{c}_0^\dagger|0\rangle\right] \tag{2.8}$$

Now, we can put (2.7) and (2.8) togheter and write:

$$\begin{aligned} H\phi_k = \left[- t\left(e^{ik}+e^{-ik}\right)+h\right]\sum_{j=1}^{L-1}\left[ae^{ikj}+be^{-ikj}\right]\hat{c}_j^\dagger|0\rangle + \\ + \left[- t(ae^{ik}+be^{-ik}) + u_A(ae^{ikL}+be^{-ikL}) + \mu(a+b)\right]\hat{c}_0^\dagger|0\rangle + \\ + \left[- t(ae^{ik(L-1)}+be^{-ik(L-1)}) + u_A^*(a+b) + \nu(ae^{ikL}+be^{-ikL})\right]\hat{c}_L^\dagger|0\rangle \end{aligned} \tag{2.9}$$

Now, the eigenvalues problem $H\phi_k = E_k\phi_k$ is solved if and only if:

(i) $\left[- t\left(e^{ik}+e^{-ik}\right)+h\right] = -2t\cos k + h = E_k$
(ii) $\left[- t(ae^{ik}+be^{-ik}) + u_A(ae^{ikL}+be^{-ikL}) + \mu(a+b)\right] = E_k(a+b)$
(iii) $\left[- t(ae^{ik(L-1)}+be^{-ik(L-1)}) + u_A^*(a+b) + \nu(ae^{ikL}+be^{-ikL})\right] = E_k(ae^{ikL}+be^{-ikL})$

The first condition is the usual bulk condition which yields a spectrum depending on $\cos k$ for a free particle on a lattice presented in the first section.
However both *(ii)* and *(ii)* must be satisfied; these conditions give us an equation that fixes the k' s values. This is the role boundary conditions play.
In the following, without loss of generality, we can set $h = 0$; thus *(ii)* and *(ii)* become:

$$\begin{aligned} a(\mu + te^{-ik} + u_Ae^{ikL}) + b(\mu + te^{+ik} + u_Ae^{-ikL}) = 0 \\ a(\nu e^{ikL} + te^{ik(L+1)} + u_A^*) + b(\nu e^{-ikL} + te^{-ik(L+1)} + u_A^*) = 0 \end{aligned} \tag{2.10}$$

These form a set of two homogeneous linear equations in a and b, that admit the non-trivial solution:

$$-\frac{b}{a} = \frac{\mu + te^{-ik} + u_Ae^{ikL}}{\mu + te^{ik} + u_Ae^{-ikL}} = \frac{\nu e^{ikL} + te^{ik(L+1)} + u_A^*}{\nu e^{-ikL} + te^{-ik(L+1)} + u_A^*} \tag{2.11}$$

only if the determinant is zero. This condition is satisfied if:

$$e^{2ikL} = \frac{\mu + te^{-ik} + u_A e^{ikL}}{\mu + te^{ik} + u_A e^{-ikL}} \cdot \frac{\nu + te^{-ik} + u_A^* e^{ikL}}{\nu + te^{ik} + u_A^* e^{-ikL}} \tag{2.12}$$

As already said, (2.12) fixes the values of k's , that are considered belonging to the range $[0, \pi]$ [3]. We notice that the r.h.s. of (2.12) yields a pure phase factor, i.e. $k \in \mathbb{R}$ if and only if:

(a) $u_A = u_A^* \Rightarrow u_A \in \mathbb{R}$.

(b) $\mu = \nu \ \ \forall\, u_A \ \in \ \mathbb{C}$.

In this case wave functions are standard superpositions of plane waves (scattering states). For more general boundary conditions, the r.h.s. of (2.12) might become a generic complex number. As we will see with some examples below, it is possible to find solution with complex k's values, which correspond to wave functions exponentially decaying from the boundaries (edge states). Some easy limits can be useful to understand all the process.

- $\boxed{\mu = \nu = 0 \ , \ u_A = u_A^* = -t}$ *Periodic Boundary conditions*

  Imposing these conditions (2.12) is fullfilled for all k such that:

  $$e^{ik(L+1)} = 1 \quad \Rightarrow \quad k_n = \frac{2n\pi}{L+1} \ , \ n = 0, 1, .., L$$

  Hence, the solutions are given by linear combinations of $\phi_n = \frac{1}{\sqrt{L+1}} e^{ik_n j}$.

- $\boxed{u_A = 0}$ *Truncated at the edge*
  In this situation, equation (2.12) becomes

  $$e^{2ikL} = \frac{\mu + te^{-ik}}{\mu + te^{ik}} \cdot \frac{\nu + te^{-ik}}{\nu + te^{ik}} = \\ = \frac{\mu\nu + t(\mu+\nu)e^{-ik} + t^2 e^{-2ik}}{\mu\nu + t(\mu+\nu)e^{ik} + t^2 e^{2ik}}$$

  In particular

  (i) if $\mu \to \infty$ or $\nu \to \infty$, we have *Dirichlet* conditions. In fact:

  $$e^{2ikL} = -\frac{b}{a} = 1 \quad \Rightarrow \quad k_n = \frac{\pi}{L} n \quad n = 1, ...L-1$$

[3] We are not taking in account all the first Brillouin zone, because the energy is symmetric for $k \to -k$ and the lattice step is $a = 1$.

The solutions are[4] $L-1$, provided by the orthonormal eigenvectors

$$\phi_n = \sqrt{\frac{2}{L+1}} \sin k_n$$

(ii) if $\mu = \nu = -t$ we have, instead, *Neumann* conditions, implying

$$e^{2ikL} = -e^{-2ik} \quad \Rightarrow \quad e^{2ik(L+1)} = 1$$
$$\Rightarrow k_n = \frac{\pi}{L+1} n \quad n = 0, ...L-1$$

In this case we have L solutions given by the eigenvectors

$$\phi_n = \frac{1}{\sqrt{L+1}} \left[e^{ik_n} - e^{-ik_n} e^{ik} \right]$$

As already mentioned, for k fixed at $k = 0$ and $k = \pi$, which are stationary points for the energy, (2.10) is satisfied also for complex values of $k's$, that could give rise to real eigenfunctions for the edge states. There are two cases:

(A) *Edge Uniform States* :

$$\boxed{k = i\alpha} \Rightarrow \phi_j = (ae^{\alpha j} + be^{-\alpha j})\hat{c}_j^\dagger |0\rangle$$
$$\Rightarrow E_\alpha = -2t(e^\alpha + e^{-\alpha})$$

(B) *Edge Staggered States*:

$$\boxed{k = \pi + i\alpha} \Rightarrow \phi_j = (-1)^j (ae^{\alpha j} + be^{-\alpha j})\hat{c}_j^\dagger |0\rangle$$
$$\Rightarrow E_\alpha = +2t(e^\alpha + e^{-\alpha})$$

These states are called staggered because of the factor $(-1)^j$, which flips the sign of the eigenfunctions site by site. This will be clear in the next section, where we are going to draw the solutions.

We remark that, for this kind of solutions, equation (2.12) becomes :

$$e^{-2\alpha L} = \frac{\mu + te^\alpha + u_A e^{-\alpha L}}{\mu + te^{-\alpha} + u_A e^{\alpha L}} \cdot \frac{\nu + te^\alpha + u_A^* e^{-\alpha L}}{\nu + te^{-\alpha} + u_A^* e^{\alpha L}} \tag{2.13}$$

We are going to analyze this situation in the continuum limit, where the role of the parameters at the edge is exactly connected to self-adjoint extensions of the Hamiltonian, and some semplifications are permitted.

[4]They are only L-1 because the two ends point do not partecipate at the total current. There is no hopping between the two edge sites.

2.2 Continuum Limit

As explained in the first chapter, a self-adjoint extension of H at the boundary is given only if exists a 2x2 unitary matrix U such that

$$\begin{pmatrix} -\dot{\phi}(0) \\ \dot{\phi}(L) \end{pmatrix} = -i\frac{\mathbb{I}+U}{\mathbb{I}-U}\begin{pmatrix} \phi(0) \\ \phi(L) \end{pmatrix} \tag{2.14}$$

In the continuum limit, our ansatz of solution is $\phi_k(x) = ae^{ikx} + be^{-ikx}$.
Let us impose

$$A = -i\frac{\mathbb{I}+U}{\mathbb{I}-U} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \tag{2.15}$$

that satisfied $A = A^\dagger$, being self-adjoint. Equation (2.14) is translated into the following system of equations:

$$\begin{aligned} a\left[-ik - a_{11} - a_{12}e^{ikL}\right] + b\left[ik - a_{11} - a_{12}e^{-ikL}\right] = 0 \\ ae^{2ikl}\left[ik - a_{22} - a_{21}e^{-ikL}\right] + b\left[-ik - a_{22} - a_{21}e^{ikL}\right] = 0 \end{aligned}$$

The crucial point, now, is to make a comparison between these equations and (2.10)[5]. Actually, moving from the discrete case to the continuous one, we have [6]:

$$\begin{aligned} a \to 0 \quad &\Rightarrow \quad e^{ika} \simeq 1 + ika \\ &\Rightarrow \quad \cos ka \simeq 1 + \frac{(ka)^2}{2} \\ &\Rightarrow \quad \sin ka \simeq ka \end{aligned}$$

Then

$$A = \quad -i\frac{\mathbb{I}+\mathbb{U}}{\mathbb{I}-\mathbb{U}} = \quad \begin{pmatrix} 1-\mu & -u_A \\ -u_A^* & 1-\nu \end{pmatrix}$$

It is now clear in which way edge parameters provide different self-adjoint extensions of the continuous Laplacian.
In this limit, equation (2.13) can be approximated to

$$e^{-2\alpha L} = \frac{\mu + e^\alpha}{u_A e^{\alpha L}} \cdot \frac{\nu + e^\alpha}{u_A^* e^{\alpha L}} \tag{2.16}$$

where we have preserved the dominating terms on the r.h.s.. It follows that

$$e^{2\alpha} + (\mu+\nu)e^\alpha + (\mu\nu - |u_A|^2) = 0 \tag{2.17}$$

[5]Let us impose $t = 1$ for sake of semplicity.

[6]We have consider a lattice step $a = 1$ in the previous section. $\mathbf{l} = (L+1)a$ is the lenght of our chain and it is fixed.

that is resolved by

$$\begin{aligned} e^{\alpha} =& \frac{-(\mu+\nu) \pm \sqrt{(\mu+\nu)^2 - 4(\mu\nu - |u_A|^2)}}{2} = \\ =& \frac{-(\mu+\nu) \pm \sqrt{(\mu-\nu)^2 + 4|u_A|^2}}{2} \end{aligned} \tag{2.18}$$

In order to have a bound state, of course, it is necessary[7] that $e^{\alpha} \geq 1$ which means

$$\pm\sqrt{(\mu-\nu)^2 + 4|u_A|^2} \geq 2 + (\mu+\nu) \tag{2.19}$$

Two regions come out:

(1) $2 + (\mu+\nu) \geq 0$ i.e. $\nu \geq -2 - \mu$

$$\begin{aligned} &\Rightarrow \sqrt{(\mu-\nu)^2 + 4|u_A|^2} \geq 2 + (\mu+\nu) \\ &\Rightarrow |u_A|^2 \geq \mu\nu + (\mu+\nu) + 1 \end{aligned} \tag{2.20}$$

while

$$\Rightarrow \quad -\sqrt{(\mu-\nu)^2 + 4|u_A|^2} \geq 2 + (\mu+\nu) \tag{2.21}$$

is never satisfied. It means that we have only one edge state:

$$e^{\alpha} = \frac{-(\mu+\nu) + \sqrt{(\mu+\nu)^2 - 4(\mu\nu - |u_A|^2)}}{2} \tag{2.22}$$

(2) $2 + (\mu+\nu) \leq 0$ i.e. $\nu \leq -2 - \mu$

$$\begin{aligned} &\Rightarrow \sqrt{(\mu-\nu)^2 + 4|u_A|^2} \leq -2 - (\mu+\nu) \\ &\Rightarrow |u_A|^2 \leq \mu\nu + (\mu+\nu) + 1 \end{aligned} \tag{2.23}$$

For staggered edge states, instead, we have:

$$e^{2\alpha} - (\mu+\nu)e^{\alpha} + (\mu\nu - |u_A|^2) = 0 \tag{2.24}$$

whose solutions are given by

$$\begin{aligned} e^{\alpha} =& \frac{(\mu+\nu) \pm \sqrt{(\mu+\nu)^2 - 4(\mu\nu - |u_A|^2)}}{2} = \\ =& \frac{(\mu+\nu) \pm \sqrt{(\mu-\nu)^2 + 4|u_A|^2}}{2} \end{aligned} \tag{2.25}$$

[7] If $e^{\alpha} < 1$ the roles of a and b are exchanged.

Imposing again $e^{\alpha} \geq 1$, we obtain

$$\pm\sqrt{(\mu-\nu)^2+4|u_A|^2} \geq 2-(\mu+\nu) \tag{2.26}$$

and the two regions are given by:

(1) $2-(\mu+\nu) \geq 0$ i.e. $\nu \leq 2-\mu$

(2) $2-(\mu+\nu) \leq 0$ i.e. $\nu \geq 2-\mu$

Once again in the first region we have only one edge state, while in the second region there are two solutions.
Let us consider first the case $\boxed{u_A = 0}$.
Now, equation (2.13) becomes:

$$(\mu \pm te^{\alpha})(\nu \pm te^{\alpha}) \simeq 0 \tag{2.27}$$

We have always two solutions. Specifically, for $k = 0$, one solution is given by :

$$e^{\alpha} = -\frac{\mu}{t} \quad \Rightarrow \quad \phi_{\alpha}(x) \propto e^{-\alpha x}$$

which gives an edge state localizaed at the left edge ($x = 0$). The other solution, instead, is provided by:

$$e^{\alpha} = -\frac{\nu}{t} \quad \Rightarrow \quad \phi_{\alpha}(x) \propto e^{-\alpha x}e^{-\alpha L}$$

that is localized at the right edge ($x = L$). Analogue considerations can be carried on for $k = \pi$.
We conclude that if $u_A = 0$, edge states are described by a real wave function that decays in an exponential way indipendently from either one of the two edge sites but depending on the strenght of μ and ν. This is illustrated in Figure (2.2)

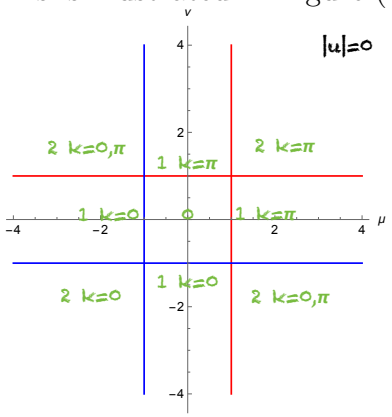


Figure 2.1: Phase diagram of Edge States for $u_A = 0.0$

When we turn on u_A, a probability current is established between the two edges and these modes are no longer indipendent, still they can decay either in a uniform or staggered way. Moreover, the region of the parameter that allow for edge states gets enlarged as we can see in Figure 2.2

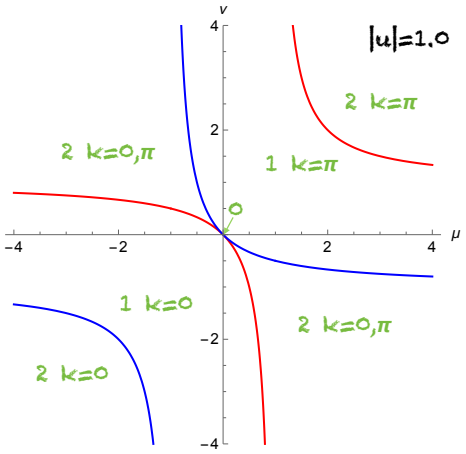


Figure 2.2: Phase diagram of Edge States for $u_A = 1.0$

In the following, we report the behaviour of the edge state wave functions for some value of u_A, μ, ν that exemplify the various case we have discussed up to now. The graphs are the result of a numerical analysis performed on a chain of 200 sites, done with Mathematica.

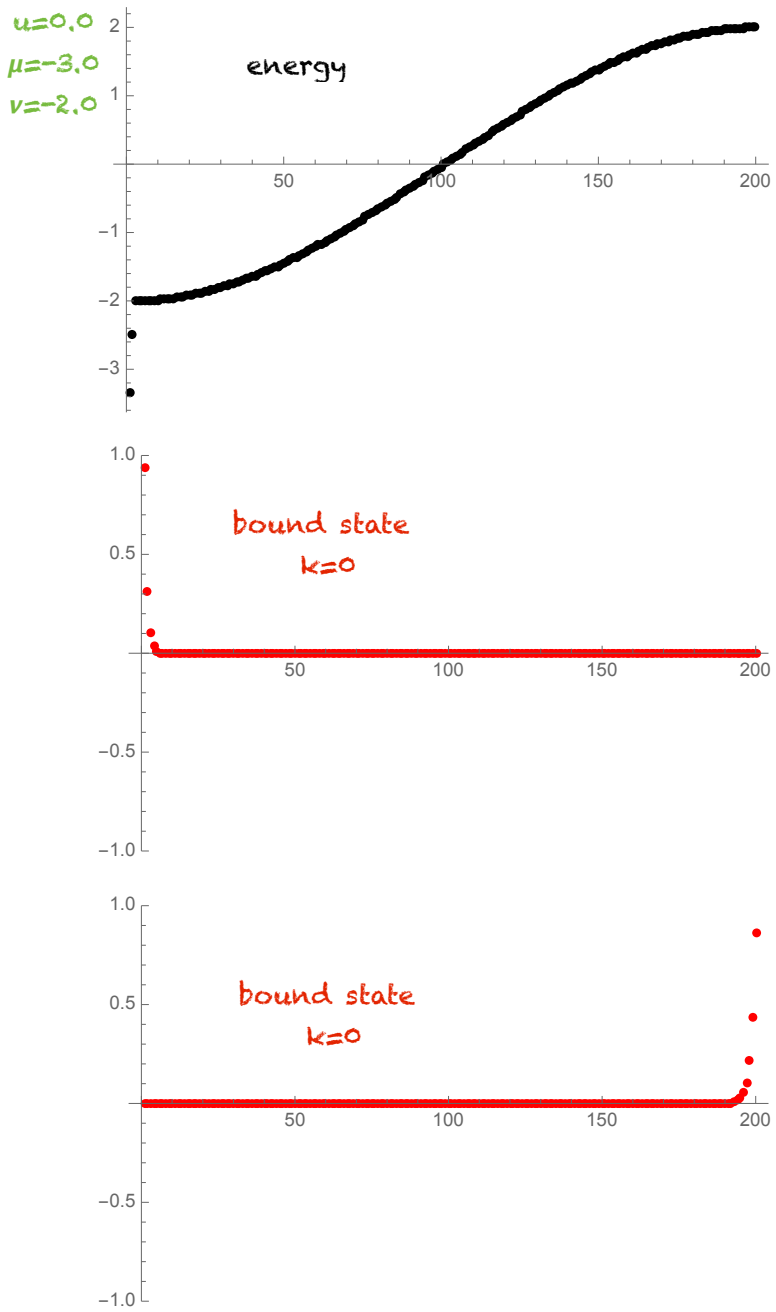


Figure 2.3: For $u_A = 0$ and μ, $\nu \leq -2$, only uniform edge states are possible, as predicted by the phase diagram of Figure 2.2. Since both μ and ν are smaller than -2, we have two uniform edge states. Wave functions can be chosen to be real; hence, the nature of these edge states is that one of Majorana modes in the Kitaev chain.

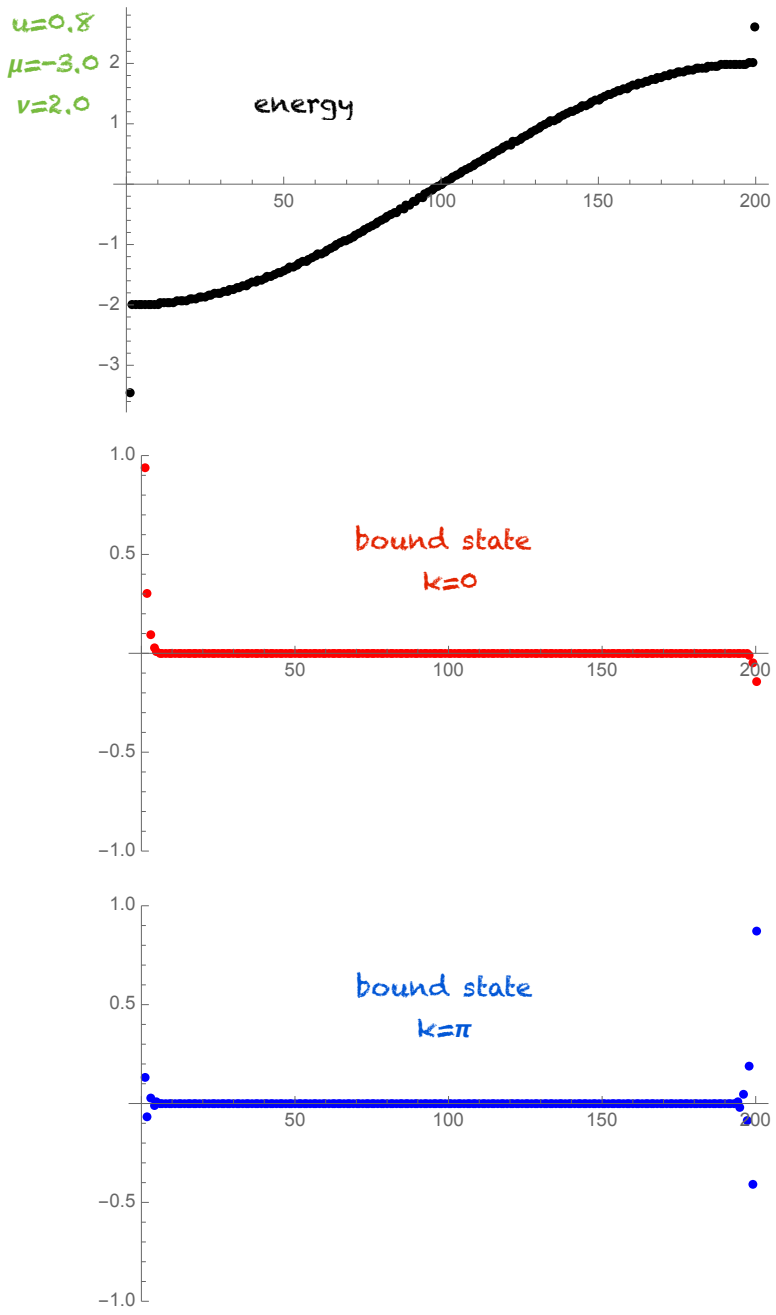
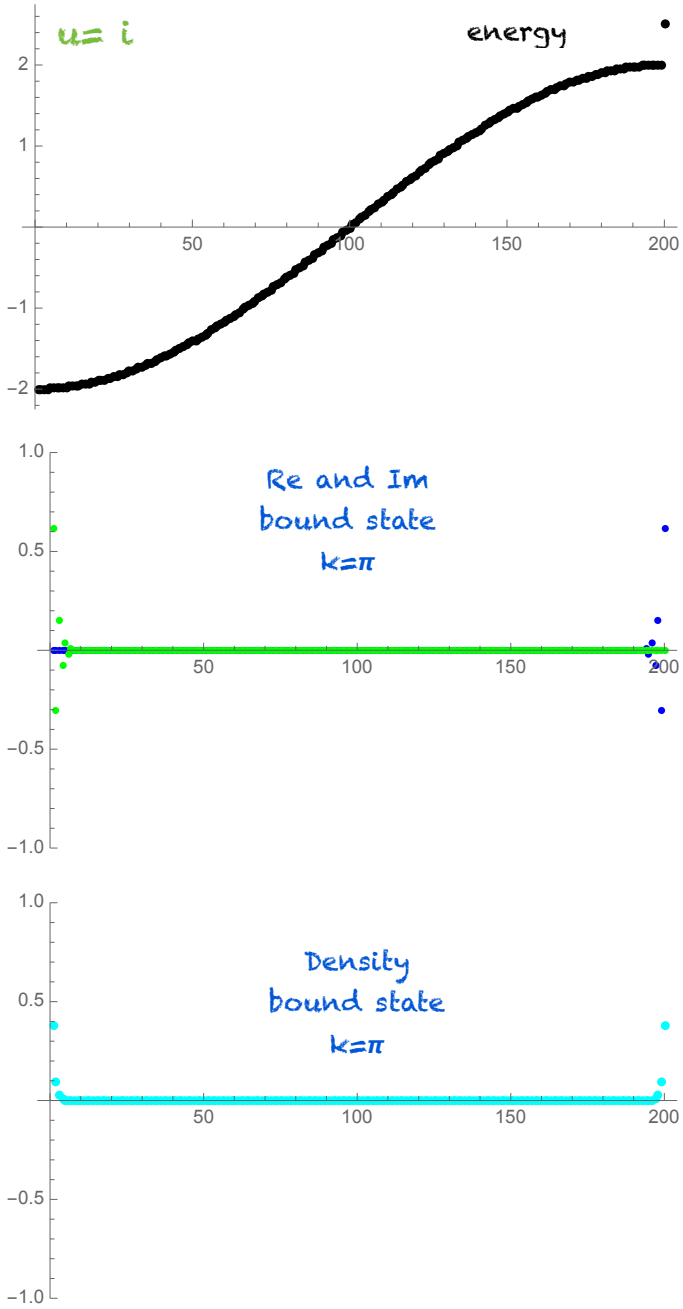


Figure 2.4: For real u_A , since $\mu \leq -2$ we have a uniform edge state bound at $x = 0$ .On the other end, because of $\nu > 2$ a staggered edge state is bound at x=L. Again wave unctions can be chosen to be real, representing a Majorana mode.



10cm

Figure 2.5: For a complex hopping parameter u_A, edge states are described by a necessary complex wave function, which decay from both ends. This means that edge states are now Dirac-like and not Majorana.

Chapter 3

Lieb - Shultz - Mattis Method

Our goal is to extend what we have done in the previous chapter for electrons interacting by a quadratic potential, similar to the Bradley-Cooper-Schrieffer potential[6] that describes the microscopic theory of superconductivity.
The Hamiltonian of the BCS-model, having already performed a Fourier transform, is given by:

$$H_{BCS} = \sum_{k\sigma}(\epsilon_k - h)\hat{c}^\dagger_{k\sigma}\hat{c}_{k\sigma} - \sum_k \left[\Delta^* \hat{c}^\dagger_{-k\downarrow}\hat{c}^\dagger_{k\uparrow} - \Delta \hat{c}_{k\uparrow}\hat{c}_{-k\downarrow}\right]$$

where ϵ_k gives the spectrum energy of free electrons properly renormalized by the coulombian interaction between them and h is the chemical potential; the Δ terms gives instead the quadratic interaction between electrons of opposite spins, estimated through the Hartree-Fock approximation considering the interaction with the phonon. Usually, H_{BCS} is diagonalize through tha so-called Bogolyubov unitary transformation

$$\begin{pmatrix} b_{k\uparrow} \\ b^\dagger_{-k\downarrow} \end{pmatrix} = U \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix}$$

for which $H_{BCS} = \sum_{k,\sigma=\uparrow,\downarrow} E_k \hat{b}^\dagger_{k\sigma}\hat{b}_{k\sigma}$; it becomes a free fermionic Hamiltonian in the new annihilation and creation operators, whose eigenvalues are provided by:

$$E_k = \pm\sqrt{(\epsilon_k - h)^2 + |\Delta|^2} \tag{3.1}$$

However, in the BCS-model, Fourier and Bogolyubov transformations are carried out in periodic boundary conditions. If we want to consider all the possible conditions, we may find a more general procedure to diagonalize a quadratic Hamiltonian with $\hat{c}^\dagger\hat{c}^\dagger$ terms, in such a way we can treat the edge sites.
Furthermore, let us notice that in the BCS theory of superconductivity are considered only interactions between fermions of opposite spin and momentum; in the following,

we are not going to take in account the spin degree of freedom, so that we are going to drop out the approximation that only electrons with opposite momentum interact. Lieb, Shultz and Mattis in 1961 provided a new general method to diagonalize an Hamiltonian with real quadratic interactions. Hence, the goal of this chapter will be extending it for complex operators in order to recover a BCS-like model.
Similarly, the same procedure is carried out studying some *spin* $\frac{1}{2}$ models , such as the XY model, for which the original spin interaction Hamiltonian can be re-written as a quadratic Hamiltonian in fermionic degrees of freedom, thanks to the Jordan-Wigner transformation[11].

3.1 Lieb-Shultz-Mattis method for Real Operators

The most general fermionic Hamiltonian on a 1-D lattice with quadratic interactions is given by:

$$H = \sum_{ij} c_i^\dagger A_{ij} c_j + \frac{1}{2}\left(c_i^\dagger B_{ij} c_j^\dagger + h.c.\right) \tag{3.2}$$

where the c_i 's and the $c_i^\dagger$'s are Fermi annihilation and creation operators. The hermicity of H requires that **A** is a symmetric matrix, while the anticommutation rules among the the c_i 's require that **B** is an antysymmetric matrix. Namely:

(i) $A_{ij} = A_{ji}$;

(ii) $B_{ij} = -B_{ji}$.

In order to diagonalize H, we are searching for a transformation:

$$\eta_k = \sum_i g_{ki} c_i + h_{ki} c_i^\dagger \eta_k^\dagger = \sum_i g_{ki} c_i^\dagger + h_{ki} c_i \tag{3.3}$$

that can be more briefly illustrated as:

$$U = \begin{pmatrix} G & H \\ H & G \end{pmatrix} \tag{3.4}$$

Let us underline that U must consists, in some way, both of Fourier transforms and Bogolyubov ones, so that we can diagonalize the Hamiltonian in the momentum space. More clearly:

- i represents the site index, so it is related to the Fourier transform that maps to the momentum space;
- k is the impulse index, upon which the Bogolyubov transform acts.

The Fourier transform is not so obvious when boundary conditions are applied. This is the reason why we are considering general transformation. The transformation U is unitary only if it preserves the anticommutation rules of the fermionic operator c_i and $c_i^\dagger$. This request means that

(i) $\{\eta_q, \eta_k\} = 0$;

(ii) $\left\{\eta_q, \eta_k^\dagger\right\} = \delta_{kq}$.

Substituing the definition of the new annihilation and creation operators in the anticommutation rules, it is simple to see that:

(i) implies $GH^T + HG^T = 0$;

(ii) implies $GG^T + HH^T = \mathbb{I}$

Moreover, the unitary transformation (3.3) makes H diagonal, i.e.

$$H = \sum_k \eta_k^\dagger \eta_k \; + \; const \tag{3.5}$$

only if:

$$[\eta_k, H] \; = \; \Lambda_k \; \eta_k \tag{3.6}$$

where the Λ_k are the energy eigenvalues related to the new operators. We have

$$\begin{aligned}[\eta_k, H] = \left[\eta_k, \sum_q \Lambda_q \eta_q^\dagger \eta_q \right] = \sum_q \; \Lambda_q \left[\eta_k, \eta_q^\dagger \eta_q\right] = \\ = \sum_q \; \Lambda_q \left(\eta_q^\dagger \left[\eta_k, \eta_q\right] \; + \; \left[\eta_k, \eta_q^\dagger\right] \eta_q\right) = \sum_q \Lambda_q \delta_{qk} \eta_k = \Lambda_k \eta_k\end{aligned}$$

Including the definitions of the new operator, it means that

$$\begin{aligned}[\eta_k, H] \; = \; \sum_{il} \; [\quad g_{ki} A_{il} \; - \; h_{ki} B_{il}] \; c_l \; + \\ + \sum_{il} [- \; h_{ki} A_{il} \; + \; g_{ki} B_{il}] \; c_l^\dagger\end{aligned} \tag{3.7}$$

From (2.5) , using the definition of η_m, these two equalities come out to be:

$$\Lambda_k g_{kl} = \sum_i \left(g_{ki} A_{il} - \; h_{ki} B_{il}\right) \tag{3.8}$$

$$\Lambda_k h_{kl} = \sum_i (-\ h_{ki} A_{il} + \ g_{ki} B_{il}) \tag{3.9}$$

It is quite simple to see that the eigenvalue problem can be resolved through the following linear combinations:

$$\psi_k = \sum_l (g_{kl} + h_{kl}) \tag{3.10}$$

$$\phi_k = \sum_l (g_{kl} - h_{kl}) \tag{3.11}$$

In fact, adding up and subttracting both sides of equations (3.8) and (3.9), we achieve:

$$\Lambda_k \psi_k = \sum_{il} \left[(g_{ki} - h_{ki})\, A_{il} + (g_{ki} - h_{ki})\, B \right] = \phi_k \left[A + B \right] \tag{3.12}$$

$$\Lambda_k \phi_k = \sum_{il} \left[(g_{ki} + h_{ki})\, A_{il} - (g_{ki} + h_{ki})\, B_{il} \right] = \psi_k \left[A - B \right] \tag{3.13}$$

Hence, we have

$$\Lambda_k^2 \psi_k = \Lambda_k \Lambda_k \psi_k = \Lambda_k \phi_k \left[A + B \right] = \psi_k \left[A - B \right] \left[A + B \right] \tag{3.14}$$

and, in the same way:

$$\Lambda_k^2 \phi_k = \Lambda_k \Lambda_k \phi_k = \Lambda_k \psi_k \left[A - B \right] = \phi_k \left[A + B \right] \left[A - B \right] \tag{3.15}$$

Thus, the problem of finding the energy spectrum Λ_k^2 is translated into the problem of finding the eigenvalues of the matrix $(\mathbf{A} + \mathbf{B})(\mathbf{A} - \mathbf{B})$

3.2 Extension to Complex Operators

In this section we want to propose an extension of Lieb-Shultz-Mattis technique to complex matrices **A** and **B**.
In this case the hermicity of H imposes that **A** is a hermitian matrix, while the anticommutation rules among the the c_i 's need **B** to be an antyhermitian matrix. Precisely:

(i) $A_{ij} = A_{ji}^*$;

(ii) $B_{ij} = -B_{ji}^*$.

So, we can rewrite our Hamiltonian in this way:

$$H = \sum_{jl} \left[\ c_j^\dagger A_{jl} c_l \ + \ c_j^\dagger \frac{B_{jl}}{2} c_l^\dagger \ - \ c_l \frac{B_{jl}^*}{2} c_j \ \right]$$

It will be clear later why we have choose to consider $\frac{1}{2}\mathbf{B}$ instead of $\mathbf{B}$. The coefficients of our transformation now have to be complex, because a complex Fourier transform is needed. Namely:

$$\begin{aligned} \eta_k &= \sum_i g_{ki} c_i + h_{ki} c_i^\dagger \\ \eta_k^\dagger &= \sum_i g_{ki}^* c_i^\dagger + h_{ki}^* c_i \end{aligned} \quad \Rightarrow \quad U = \begin{pmatrix} G & H \\ H^* & G^* \end{pmatrix} \tag{3.16}$$

The preservation of the anticommutation rules of the fermionic operator c_i and $c_i^\dagger$ in this situation are such that

- $\{\eta_q, \eta_k\} = 0$ implies $GH^\dagger + HG^\dagger = 0$;
- $\left\{\eta_q, \eta_k^\dagger\right\} = \delta_{kq}$ implies $GG^T + HH^T = \mathbb{I}$

Let us see at one of these relations as an example:

$$\begin{aligned} \{\eta_q, \eta_k^\dagger\} &= \left\{ \sum_i g_{qi}\ c_i + \ h_{qi}\ c_i^\dagger\ ,\ \sum_j h_{kj}^*\ c_j + \ g_{kj}^*\ c_j^\dagger \right\} = \\ &= \sum_{i,j} \left[g_{qi} h_{kj}^* \{c_i, c_j\} + g_{qi} g_{kj}^* \{c_i, c_j^\dagger\} + h_{qi} h_{kj}^* \{c_i^\dagger, c_j\} + h_{qi} g_{kj}^* \{c_i^\dagger, c_j^\dagger\} \right] = \\ &= \sum_{i,j} \left[g_{qi} g_{kj}^* \delta_{ij} \ + \ h_{qi} h_{kj}^* \delta_{ij} \right] = \sum_i \left[g_{qi} g_{ki}^* \ + \ h_{qi} h_{ki}^* \right] \ = \\ &= \left(GG^\dagger \ + \ HH^\dagger \right)_{qk} \end{aligned}$$

We have to impose that (3.16) diagonalizes H, i.e. $[\eta_k, H] \ = \ \Lambda_k\ \eta_k$.
Let us evaluate first $[\eta_k, H]$:

$$\begin{aligned} [\eta_k, H] = &\sum_{ijl} g_{ki} A_{jl}\ [c_i\ ,\ c_j^\dagger c_l] \ + \sum_{ijl} h_{ki} A_{jl}\ [c_i^\dagger\ ,\ c_j^\dagger c_l] \ + \\ &+ \sum_{ijl} g_{ki} \frac{B_{jl}}{2}\ [c_i\ ,\ c_j^\dagger c_l^\dagger] \ + \ \sum_{ijl} h_{ki} \frac{B_{jl}}{2}\ [c_i^\dagger\ ,\ c_j^\dagger c_l^\dagger] \ + \\ &- \sum_{ijl} g_{ki} \frac{B_{lj}^*}{2}\ [c_i\ ,\ c_l c_j] \ - \sum_{ijl} h_{ki} \frac{B_{lj}^*}{2}\ [c_i^\dagger\ ,\ c_l c_j] \end{aligned}$$

that, making use of the properties of our operators $\mathbf{A}$ and $\mathbf{B}$, becomes

$$\begin{aligned} [\eta_k, H] \ = \ &\sum_{il} \left[\ \ g_{ki} A_{il} \ - \ h_{ki} \frac{B_{il} + B_{il}^*}{2} \right] \ c_l \ + \\ &+ \sum_{il} \left[- \ h_{ki} A_{il}^* \ + \ g_{ki} \frac{B_{il} + B_{il}^*}{2} \right] \ c_l^\dagger \end{aligned} \tag{3.17}$$

Let us impose $\tilde{B}_{ij} = \frac{B_{il}+B^*_{il}}{2} = Re[B_{ij}]$ and notice that just the real part of $\mathbf{B}$ has an effective role in the dynamics of the new particles describes by η_k, $\eta^\dagger_k$.
Then, if our transformation makes H diagonal, the following equalities must be satisfied:

$$\Lambda_k g_{kl} = \sum_i \Big(g_{ki} A_{il} - \ h_{ki} \tilde{B}_{il} \Big) \tag{3.18}$$

$$\Lambda_k h_{kl} = \sum_i \Big(- \ h_{ki} A^*_{il} + \ g_{ki} \tilde{B}_{il} \Big) \tag{3.19}$$

It is time to explicitly express the hamiltonian terms; we will work with a traslational invariant Hamiltonian in the nearest neighbours approximation; hence, let us consider hopping and interaction elements complex, which relate nearest neghbours sites.
Let us take them the same for all of the sites[1]:

$$\begin{cases} A_{l-1,l} = A e^{-i\phi} \\ A_{l+1,l} = A^*_{l,l+1} = A e^{i\phi} \end{cases} \tag{3.20}$$

Moreover $A_{l,l}$ will simply be the chemical potential.

$$\begin{cases} B_{l-1,l} = \Delta_0 e^{i\theta} \\ B_{l+1,l} = -B^*_{l,l+1} = \Delta_0 e^{-i\theta} \end{cases} \quad \Rightarrow \quad \begin{cases} \tilde{B}_{l+1,l} = -\Delta_0 \cos\theta \\ \tilde{B}_{l-1,l} = \ \Delta_0 \cos\theta \end{cases} \tag{3.21}$$

Thanks to the translational invariance away from the edge, we can suggest an ansatz of solutions in terms of plane waves:

$$\begin{cases} g_{kl} = a_k e^{ikl} + b_k e^{-ikl} \\ h_{kl} = c_k e^{ikl} + d_k e^{-ikl} \end{cases} \tag{3.22}$$

Now, according to the nearest neighbours approximation, the r.h.s. of equation (3.18) includes only five elements:

$$\begin{aligned} \Lambda_k g_{kl} = g_{k(l+1)} A_{l+1,l} + g_{kl} A_{l,l} + g_{k(l-1)} A_{l-1,l} + \\ - \ h_{k(l+1)} \tilde{B}_{l+1,l} - h_{k(l-1)} \tilde{B}_{l-1,l} \end{aligned}$$

that means

$$\begin{aligned} (\Lambda_k - A_{l,l}) \left(a_k e^{ikl} + b_k e^{-ikl} \right) = \left(a_k e^{ik(l+1)} + b_k e^{-ik(l+1)} \right) A e^{i\phi} + \left(a_k e^{ik(l-1)} + b_k e^{-ik(l-1)} \right) A e^{-i\phi} + \\ - \left(c_k e^{ik(l+1)} + d_k e^{-ik(l+1)} \right) (-\Delta_0 \cos\theta) + \\ - \left(c_k e^{ik(l-1)} + d_k e^{-ik(l-1)} \right) (\Delta_0 \cos\theta) \end{aligned}$$

It is then possible to separate the real and the imaginary part of e^{ikl}, namely:

$$e^{ikl} = \cos(kl) + i \sin(kl)$$

[1] It is implicit that we are working with a U(1) global symmetry.

so that we can easily derive two equations from (3.18):

- one for $\underline{\cos(kl)}$

$$\begin{aligned}(\Lambda_k - A_{l,l})\,(a_k + b_k) =& 2A\cos(k+\phi)\; a_k + \; 2A\cos(k-\phi)\; b_k + \\ &+ 2i\Delta_0\cos\theta\sin k\; c_k - \; 2i\Delta_0\cos\theta\sin k\; d_k\end{aligned} \tag{3.23}$$

- and another for $\underline{i\sin(kl)}$

$$\begin{aligned}(\Lambda_k - A_{l,l})\,(a_k - b_k) =& 2A\cos(k+\phi)\; a_k - \; 2A\cos(k-\phi)\; b_k + \\ &+ 2i\Delta_0\cos\theta\sin k\; c_k + \; 2i\Delta_0\cos\theta\sin k\; d_k\end{aligned} \tag{3.24}$$

The combinations (3.23) $\pm$ (3.24) provides us two equations where it is clear that the four coefficients of our anstatz are related two by two:

$$(\Lambda_k - A_{l,l})\; a_k = 2A\cos(k+\phi)\; a_k + 2i\Delta_0\cos\theta\sin k\; c_k \tag{3.25}$$

$$(\Lambda_k - A_{l,l})\; b_k = 2A\cos(k-\phi)\; b_k - 2i\Delta_0\cos\theta\sin k\; d_k \tag{3.26}$$

Repeating the same procedure for (3.9), with the precaution that $A^*_{l,l} = A_{l,l}$ because of the hermicity of $\mathbf{A}$, we obtain:

$$(\Lambda_k + A_{l,l})\; c_k = -2A\cos(k-\phi)\; c_k - 2i\Delta_0\cos\theta\sin k\; a_k \tag{3.27}$$

$$(\Lambda_k + A_{l,l})\; d_k = -\; 2A\cos(k+\phi)\; d_k + 2i\Delta_0\cos\theta\sin k\; b_k \tag{3.28}$$

In conlusion we end up with four equations:

$$\begin{aligned}(\Lambda_k - A_{l,l})\; a_k &= 2A\cos(k+\phi)\; a_k + 2i\Delta_0\cos\theta\sin k\; c_k \\ (\Lambda_k - A_{l,l})\; b_k &= 2A\cos(k-\phi)\; b_k - 2i\Delta_0\cos\theta\sin k\; d_k \\ (\Lambda_k + A_{l,l})\; c_k &= -2A\cos(k-\phi)\; c_k - 2i\Delta_0\cos\theta\sin k\; a_k \\ (\Lambda_k + A_{l,l})\; d_k &= -2A\cos(k+\phi)\; d_k + 2i\Delta_0\cos\theta\sin k\; b_k\end{aligned} \tag{3.29}$$

Making use of the trigonometric relation

$$\cos(\alpha \pm \beta) = \cos\alpha\cos\beta \mp \sin\alpha\sin\beta$$

and defining

- $2A\cos k\cos\phi = R$
- $2A\sin k\sin\phi = T$
- $2i\Delta_0\cos\theta\sin k = I$

the system of equations (3.29) becomes:

$$\begin{aligned}(\Lambda_k - A_{l,l})\; a_k &= (R-T)\; a_k + \; I\; c_k \\ (\Lambda_k - A_{l,l})\; b_k &= (R+T)\; b_k - \; I\; d_k \\ (\Lambda_k + A_{l,l})\; c_k &= -(R+T)\; c_k - \; I\; a_k \\ (\Lambda_k + A_{l,l})\; d_k &= -(R-T)\; d_k + \; I\; b_k\end{aligned} \tag{3.30}$$

3.2.1 Real Hopping

Let us consider the case of real hopping coefficients; if **A** is real, then $\phi = 0$ in (3.20). It follows that

$$R = 2A\cos k \qquad T = 0 \qquad I = 2i\Delta_0 \cos\theta \sin k$$

Thanks to $T = 0$, the system of four equations reduces to two identical systems of two equations.
Explicitly:

$$\begin{aligned}\Lambda_k\ (a_k \pm b_k) &= (R + A_{l,l})\ (a_k \pm b_k) + \ I\ (c_k \mp d_k)\\ \Lambda_k\ (c_k \mp d_k) &= -\,(R + A_{l,l})\ (c_k \mp d_k) - \ I\ (a_k \pm b_k)\end{aligned}$$

It is very easy to find the eigeinvalues Λ_k of the matrix:

$$N = \begin{pmatrix} \tilde{R} & I \\ -I & -\tilde{R} \end{pmatrix}$$

where $\tilde{R} = R + A_{l,l}$.
The eigenvalues are given by:

$$\begin{gathered}\left(\tilde{R} - \Lambda_k\right)\left(-\tilde{R} - \Lambda_k\right) + I^2 = 0\\ \Lambda_k^2 - \tilde{R}^2 + I^2 = 0\\ \Lambda_{k_\pm} = \pm\sqrt{\tilde{R}^2 - I^2}\end{gathered}$$

Making R and I explicit, we obtain the following eigenvalues:

$$\Lambda_{k_\pm} = \pm\sqrt{(-2A\cos k + A_{l,l})^2 + 4\Delta_0^2 \sin^2 k} \tag{3.31}$$

They are the discrete analogue of (3.1), where $A_{l,l} = -h$ and $A = -t$. To be more precise, we can find other linear combinations of $a_k,\ b_k,\ c_k,\ d_k$ to enlighten which are the eigenfunctions of the Hamiltonian; in fact if we consider:

$$\begin{aligned}\Lambda_k\ (\ a_k + c_k) &= \left(\tilde{R} - I\right)\ (\ a_k - c_k)\\ \Lambda_k\ (\ a_k - c_k) &= \left(\tilde{R} + I\right)\ (\ a_k + c_k)\\ \Lambda_k\ (\ b_k + d_k) &= \left(\tilde{R} - I\right)\ (\ b_k - d_k)\\ \Lambda_k\ (\ b_k - b_k) &= \left(\tilde{R} + I\right)\ (\ b_k + d_k)\end{aligned}$$

it is automatically clear that

$$\Lambda_k\ (\ g_{kl} \pm h_{kl}) = \left(\tilde{R} \mp I\right)\ (\ g_{kl} \mp h_{kl}) \tag{3.32}$$

So, the eigenvalue problem can be resolved through the following linear combinations:

$$\psi_k = \sum_l (g_{kl} + h_{kl}) \tag{3.33}$$

$$\phi_k = \sum_l (g_{kl} - h_{kl}) \tag{3.34}$$

In fact, equations (3.8) and (3.9), in this case of real hopping, become:

$$\Lambda_k g_{kl} = \sum_i \left(g_{ki} A_{il} - \ h_{ki} \tilde{B}_{il} \right)$$
$$\Lambda_k h_{kl} = \sum_i \left(- \ h_{ki} A_{il} + \ g_{ki} \tilde{B}_{il} \right)$$

Adding up and subtracting both sides, we achieve

$$\Lambda_k \psi_k = \sum_{il} \left[(g_{ki} - h_{ki}) A_{il} + (g_{ki} - h_{ki}) \tilde{B}_{il} \right] = \phi_k \left[A + \tilde{B} \right] \tag{3.35}$$

$$\Lambda_k \phi_k = \sum_{il} \left[(g_{ki} + h_{ki}) A_{il} - (g_{ki} + h_{ki}) \tilde{B}_{il} \right] = \psi_k \left[A - \tilde{B} \right] \tag{3.36}$$

Hence,

$$\Lambda_k^2 \psi_k = \Lambda_k \Lambda_k \psi_k = \Lambda_k \phi_k \left[A + \tilde{B} \right] = \psi_k \left[A - \tilde{B} \right] \left[A + \tilde{B} \right] \tag{3.37}$$

and, in the same way:

$$\Lambda_k^2 \phi_k = \Lambda_k \Lambda_k \phi_k = \Lambda_k \psi_k \left[A - \tilde{B} \right] = \phi_k \left[A + \tilde{B} \right] \left[A - \tilde{B} \right] \tag{3.38}$$

As expected, we recover the same set of equations of the standard LSM method.

3.2.2 Complex Hopping

Now, we want to analyze the possibility of complex hopping terms even if we will not use the results, because in two dimensional system it would be useful in order to take in account the interaction with an external magnetic field[2].
One more time, it is neccesary to start from the system of equations (3.30). The Bogolyubov coefficients are always related two by two, but now the two subsystems of two equations are no longer equal as in the real case. Let us start with the pair (a_k, c_k), described by the set of equations:

$$\begin{aligned}\Lambda_k\ a_k &= (R - T + A_{l,l})\ a_k + \ I\ c_k \\ \Lambda_k\ c_k &= -\,(R + T + A_{l,l})\ c_k - \ I\ a_k\end{aligned}$$

Having in mind the substituition $R + A_{l,l} = \tilde{R}$, it is easy to evaulate the eigeenvalues Λ_k of the matrix:

$$M = \begin{pmatrix} \tilde{R} - T & I \\ -I & -(\tilde{R} + T) \end{pmatrix}$$

From imposing the secular equation $det(M - \Lambda\mathbb{I}) = 0$, it emerges that:

$$\begin{gathered}\left(\tilde{R} - T - \Lambda_k\right)\left(-\tilde{R} - T - \Lambda_k\right) + I^2 = 0 \\ (T + \Lambda_k)^2 - \tilde{R}^2 + I^2 = 0 \Lambda_k^2 + 2\Lambda_k T + T^2 - \tilde{R}^2 + I^2 = 0 \\ \Lambda_{k_\pm} = -T \pm \sqrt{\tilde{R}^2 - I^2}\end{gathered} \tag{3.39}$$

The pair (b_k, d_k) satisfies, instead, the equations:

$$\begin{aligned}\Lambda_k\ d_k &= (R + T + A_{l,l})\ b_k - \ I\ d_k \\ \Lambda_k\ b_k &= -\,(R - T + A_{l,l})\ b_k + \ I\ d_k\end{aligned}$$

The resulting matrix is :

$$P = \begin{pmatrix} \tilde{R} + T & -I \\ I & -(\tilde{R} - T) \end{pmatrix}$$

where the same substituion $R + A_{l,l} = \tilde{R}$ has been done. Solving again the secular equation $det(P - \Lambda\mathbb{I}) = 0$, we have:

$$\begin{gathered}\left(\tilde{R} + T - \Lambda_k\right)\left(-\tilde{R} + T - \Lambda\right) + I^2 = 0 \\ (T - \Lambda)^2 - \tilde{R}^2 + I^2 = 0 \Lambda_k^2 - 2\Lambda_k T + T^2 - \tilde{R}^2 + I^2 = 0 \\ \Lambda_{k_\pm} = T \pm \sqrt{\tilde{R}^2 - I^2}\end{gathered} \tag{3.40}$$

Notice that (3.39) and (3.40) are similar except fot $T \leftrightarrow -T$. Hence, in the case of complex hopping, it is more complicated to find out which linear combinations of g_{kl}

[2]See the last chapter.

and h_{kl} can resolve our problem, because of the four different eigenvalues. Indeed, such a complex hopping gives place to different eigenvalues for the outgoing and ingoing plane waves of the Fourier transformation. Precisely, we have

$$\begin{aligned}
(\Lambda_k + T)\ a_k &= \tilde{R}\ a_k + \ I\ c_k \\
(\Lambda_k - T)\ b_k &= \tilde{R}\ b_k - \ I\ d_k \\
(\Lambda_k + T)\ c_k &= -\tilde{R}\ c_k - \ I\ a_k \\
(\Lambda_k - T)\ d_k &= -\tilde{R}\ d_k + \ I\ b_k
\end{aligned}$$

from which:

$$\begin{aligned}
(\Lambda_k + T)\,(a_k \pm c_k) &= \left(\tilde{R} \mp I\right)(a_k \mp c_k) \\
(\Lambda_k - T)\,(b_k \pm d_k) &= \left(\tilde{R} \pm I\right)(b_k \mp d_k)
\end{aligned} \tag{3.41}$$

In this way it is clear from (3.41) that a complex hopping produces an opposite shift for Bogolyubov particle of impulse k, and those ones having impulse $-k$. Λ_k is shifted of $\pm T$ respectively in the first and in the second case. This fact suggests to define the following functions [3] :

$$\begin{aligned}
\psi_{k_+} &= \sum_l (a_k + c_k)\, e^{ikl} \\
\psi_{k_-} &= \sum_l (b_k + d_k)\, e^{-ikl} \\
\phi_{k_+} &= \sum_l (a_k - c_k)\, e^{ikl} \\
\phi_{k_-} &= \sum_l (b_k - d_k)\, e^{-ikl}
\end{aligned} \tag{3.42}$$

In fact, we have:

$$(\Lambda_k + T)\,(\Lambda_k - T)\,(a_k \pm c_k)\,(b_k \pm d_k) = \left(\tilde{R} \mp I\right)\left(\tilde{R} \pm I\right)(a_k \mp c_k)\,(b_k \mp d_k)$$

Hence,

$$\left(\Lambda_k^2 - T^2\right)(a_k \pm c_k)\,(b_k \pm d_k) = \left(\tilde{R} \mp I\right)\left(\tilde{R} \pm I\right)(a_k \mp c_k)\,(b_k \mp d_k)$$

[3]The second index $\pm$ represents the sign of the impulse associated to the creation (annichilation) fermionic operator after the Fourier transformation($\hat{c}_k = \sum_l \hat{c}_l e^{ikl}$) .

We finally come to these four equations:

$$\begin{aligned}
\Lambda_k^2 (a_k + c_k)(b_k + d_k) &= \left[T^2 + \left(\tilde{R}^2 - I^2\right)\right](a_k - c_k)(b_k - d_k) \\
\Lambda_k^2 (a_k - c_k)(b_k - d_k) &= \left[T^2 + \left(\tilde{R}^2 - I^2\right)\right](a_k + c_k)(b_k + d_k) \\
\Lambda_k^2 (a_k + c_k)(b_k - d_k) &= \left[T^2 + \left(\tilde{R} - I\right)^2\right](a_k - c_k)(b_k + d_k) \\
\Lambda_k^2 (a_k - c_k)(b_k + d_k) &= \left[T^2 + \left(\tilde{R} + I\right)^2\right](a_k + c_k)(b_k - d_k)
\end{aligned}$$

These are a new set of eigenvalues equations, which generalize the real case studied in the original paper by Lieb, Shultz and Mattis. The new eigenvalue problem is resolved by the eigenfunctions of the following operators:

- $A^*A \pm 2Re[A]\tilde{B} + \tilde{B}^2$, whose eigenvalues are given by $T^2 + \left(\tilde{R} + I\right)^2$;
- $\left(A^* \pm \tilde{B}\right)\left(A \mp \tilde{B}\right)$, whose eigenvalues are provided by $T^2 + \left(\tilde{R}^2 - I^2\right)$

Thanks to this extended method, we are now ready to implement boundary conditions proceeding in the same way of the free case.

Chapter 4

Interacting case

We are going to introduce in our lattice of $L+1$ sites a BCS-like interaction bewteen nearest neighbour fermions, with the most general boundary parameters in such a way the Hamiltonian remains hermitian. Using the diagonalization through the Lieb-Shultz-Mattis method with real hopping, we can determine for which parameters edge states are allowed. We will see that interactions produce a new kind of states, called *Zero Modes*, in addition to scattering states and edge states we have found in the free case.

Our system is now described by the following Hamiltonian:

$$\begin{aligned} H = &\sum_{i=1}^{L-1}\left[-t\left(\hat{c}_{i-1}^{\dagger}\hat{c}_i + \hat{c}_{i+1}^{\dagger}\hat{c}_i\right) + h\hat{c}_i^{\dagger}\hat{c}_i\right] - t\left(\hat{c}_1^{\dagger}\hat{c}_0 + \hat{c}_{L-1}^{\dagger}\hat{c}_L\right) + \\ &+u_A\hat{c}_0^{\dagger}\hat{c}_L + u_A^*\hat{c}_L^{\dagger}\hat{c}_0 + \mu\hat{c}_0^{\dagger}\hat{c}_0 + \nu\hat{c}_L^{\dagger}\hat{c}_L + \\ &+\sum_{i=1}^{L-1}\left[\Delta\hat{c}_{i-1}^{\dagger}\hat{c}_i^{\dagger} - \Delta^*\hat{c}_{i+1}\hat{c}_i\right] + \Delta\hat{c}_{L-1}^{\dagger}\hat{c}_L^{\dagger} - \Delta^*\hat{c}_1\hat{c}_0 - u_B\hat{c}_0^{\dagger}\hat{c}_L^{\dagger} + u_B^*\hat{c}_L\hat{c}_0 \end{aligned} \tag{4.1}$$

So that

$$A = \begin{pmatrix} \mu & -t & 0 & \cdots & 0 & 0 & u_A \\ -t & h & -t & 0 & \cdots & 0 & 0 \\ 0 & -t & h & -t & 0 & \cdots & 0 \\ \vdots & & & & & & \vdots \\ 0 & \cdots & & & & -t & 0 \\ 0 & 0 & \cdots & & 0 & -t & h & -t \\ u_A^* & 0 & 0 & \cdots & 0 & -t & \nu \end{pmatrix} \qquad B = \begin{pmatrix} 0 & \Delta & 0 & \cdots & 0 & 0 & -u_B \\ -\Delta^* & 0 & \Delta & 0 & \cdots & 0 & 0 \\ 0 & -\Delta^* & 0 & \Delta & 0 & \cdots & 0 \\ \vdots & & & & & & \vdots \\ 0 & \cdots & & & & \Delta & 0 \\ 0 & 0 & \cdots & & -\Delta^* & 0 & \Delta \\ u_B^* & 0 & 0 & \cdots & 0 & -\Delta^* & 0 \end{pmatrix} \tag{4.2}$$

We have already seen with Lieb-Schultz- Mattis method how is it possible to diagonalize H. We will first examine the bulk spectrum of (4.1) and then we will discuss boundary conditions.

4.1 Bulk Spectrum

According to Lieb-Schultz-Mattis Method, our solution satisfies

$$\Lambda_k^2 \phi_k = (A + \tilde{B})(A - \tilde{B})\phi_k \tag{4.3}$$

where

$$\tilde{B} = \frac{B + B^*}{2} = \begin{pmatrix} 0 & \Delta_0 & 0 & . & . & . & 0 & 0 & -u_{0B} \\ -\Delta_0 & 0 & \Delta_0 & 0 & . & . & . & 0 & 0 \\ 0 & -\Delta_0 & 0 & \Delta_0 & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ 0 & . & . & . & . & . & . & \Delta_0 & 0 \\ 0 & 0 & . & . & . & 0 & -\Delta_0 & 0 & \Delta_0 \\ u_{0B} & 0 & 0 & . & . & . & 0 & -\Delta_0 & 0 \end{pmatrix} \tag{4.4}$$

is real. Thus:

$$\left(A + \tilde{B}\right) = \begin{pmatrix} . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ -t-\Delta_0 & h & -t+\Delta_0 & . & . & . & . \\ . & -t-\Delta_0 & h & -t+\Delta_0 & . & . & . \\ . & . & -t-\Delta_0 & h & -t+\Delta_0 & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \end{pmatrix} \tag{4.5}$$

$$\left(A - \tilde{B}\right) = \begin{pmatrix} . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ -t+\Delta_0 & h & -t-\Delta_0 & . & . & . & . \\ . & -t+\Delta_0 & h & -t-\Delta_0 & . & . & . \\ . & . & -t+\Delta_0 & h & -t-\Delta_0 & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \end{pmatrix} \tag{4.6}$$

Because of:

$$\left[\left(A + \tilde{B}\right)\left(A - \tilde{B}\right)\right]_{kl} = \left[\sum_i \left(A + \tilde{B}\right)_{ki} \left(A - \tilde{B}\right)_{i\ l}\right] \tag{4.7}$$

we obtain:

$$\left(A - \tilde{B}\right)\left(A + \tilde{B}\right) = \begin{pmatrix} . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ . & . & t^2 - \Delta_0^2 & -2ht & h^2 + 2\left(t^2 + \Delta_0^2\right) & -2ht & t^2 - \Delta_0^2 & . & . \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \end{pmatrix} \tag{4.8}$$

In (4.8) the generic form of the k-th row is shown. The diagonal element is $h^2 + 2\left(t^2 + \Delta_0^2\right)$; thus each site is connected to the subsequent and the previous two. The Hamiltonian is still translational invariant inside the bulk, so we can propose that the most general ansatz of solution is of the form:

$$\phi_k = Az^k + Bz^{-k} \tag{4.9}$$

which includes all possible types of eigenfunctions, if we allow $z \in \mathbb{C}$.
Using (4.8) and (4.9), the eigenvalues problem becomes

$$\begin{aligned} E_k^2 \left(Az^k + Bz^{-k}\right) = &\left(t^2 - \Delta_0^2\right)\left(Az^{k-2} + Bz^{-k+2}\right) + \\ &+ (-2ht)\left(Az^{k-1} + Bz^{-k+1}\right) + \\ &+ \left[h^2 + 2(t^2 + \Delta_0^2)\right]\left(Az^k \quad + Bz^{-k} \quad\right) + \\ &+ (-2ht)\left(Az^{k+1} + Bz^{-k-1}\right) + \\ &+ \left(t^2 - \Delta_0^2\right)\left(Az^{k+2} + Bz^{-k-2}\right) \end{aligned} \tag{4.10}$$

More precisely,

$$E_k^2 \left(Az^k + Bz^{-k}\right) = \left[\left(t^2 - \Delta_0^2\right)\left(z^{-2} + z^2\right) - 2ht\left(z^{-1} + z\right) + h^2 + 2\left(t^2 + \Delta_0^2\right)\right]\left(Az^k + Bz^{-k}\right)$$

Now it is easy to see that:

$$E_k^2 = \left[t\left(z^{-1} + z\right) - h\right]^2 - \Delta_0^2\left(z^{-1} - z\right)^2 \tag{4.11}$$

According to the hermicity of the Hamiltonian, the quadratic energy eigenvalues must be real. The next step, therefore, is imposing conditions of reality of the r.h.s., since in general we assume $z \in \mathbb{C}$.
In order to extract the complex part, let us define:

$$z = \lambda e^{ik} \tag{4.12}$$

with $\lambda \geq 0$. In this way :

$$\begin{aligned} (z + z^{-1}) &= \left(\lambda e^{ik} + \lambda^{-1} e^{-ik}\right) = (\lambda + \lambda^{-1})\cos k + i\,(\lambda - \lambda^{-1})\sin k \\ (z - z^{-1}) &= \left(\lambda e^{ik} - \lambda^{-1} e^{-ik}\right) = (\lambda - \lambda^{-1})\cos k + i\,(\lambda + \lambda^{-1})\sin k \end{aligned}$$

Let us also doing the following substituition in such a way to simplify the next passages:

$$\begin{aligned} (\lambda + \lambda^{-1}) &= \alpha \\ (\lambda - \lambda^{-1}) &= \beta \end{aligned} \quad \longleftrightarrow \quad \begin{aligned} \alpha + \beta &= \lambda \\ \alpha - \beta &= \lambda^{-1} \end{aligned} \tag{4.13}$$

As a consequence, (4.11) can be written as:

$$\begin{aligned} E_k^2 \;= t^2\left(\alpha^2 \cos^2 k - \beta^2 \sin^2 k\right) - 2ht\alpha \cos k + h^2 - \Delta_0^2\left(\beta^2 \cos^2 k - \alpha^2 \sin k^2\right) + \\ + 2i\beta \sin k\left[\left(t^2 - \Delta_0^2\right)\alpha \cos k - ht\right] \end{aligned} \tag{4.14}$$

Then, three are the conditions that could make the complex part of E_k^2 vanish:

(1) $\beta = \lambda - \lambda^{-1} = 0$

(2) $\sin k = 0$

(3) $(t^2 - \Delta_0^2)\,\alpha \cos k - ht = 0$

In the following we will discuss these three cases separately and show that they correspond to what we call *Scattering*, *Edge* and *Zero Mode* states, respectively.

4.1.1 Scattering States

Let us start with the first condition of reality.

$$\beta = 0 \quad \Rightarrow \quad \lambda = \lambda^{-1} \quad \Rightarrow \quad \lambda = 1 \quad \Rightarrow \quad \boxed{z = e^{ik}} \tag{4.15}$$

Hence, we have as solution a linear combination of plane waves, as expected in the bulk. In fact, from (4.15), (4.14) becomes:

$$\begin{aligned} E_k^2 \; &= t^2\alpha^2 \cos^2 k - 2ht\alpha \cos k + h^2 + \Delta_0^2\alpha^2 \sin k^2 = \\ &= \left[2t \cos k - h\right]^2 + 4\Delta_0^2 \sin k^2 \end{aligned}$$

where we have already set $\lambda = 1$ i.e. $\alpha = 2$. This is the usual dispersion relation of BCS model in a one-dimensional lattice.

$$E_{k_\pm} \; = \pm\sqrt{\left[2t \cos k - h\right]^2 + 4\Delta_0^2 \sin k^2} \tag{4.16}$$

In order to make possile a comparison with the other cases when the reality conditions is satisfied, let us analyze E_k^2 for the scattering states in function of k . Maxima and minima are provided by stationary points defined by:

$$\frac{\partial E_k^2}{\partial k} = 4 \sin k \left[ht - 2 \cos k \left(t^2 - \Delta_0^2\right)\right] = 0$$

Namely:

(a) $\sin k = 0 \quad \Leftrightarrow \quad k = 0, \pi$
corresponding to an energy

$$E_k^2\Big|_{\sin k = 0} \; = \left[\pm 2t - h\right]^2$$

(b) $\cos k = \frac{ht}{2(t^2 - \Delta_0^2)}$ whose energy is given by

$$E_k^2\Big|_{\cos k = \frac{ht}{2(t^2-\Delta_0^2)}} \; = 4\Delta_0^2 - \frac{h^2\Delta_0^2}{(t^2 - \Delta_0^2)}$$

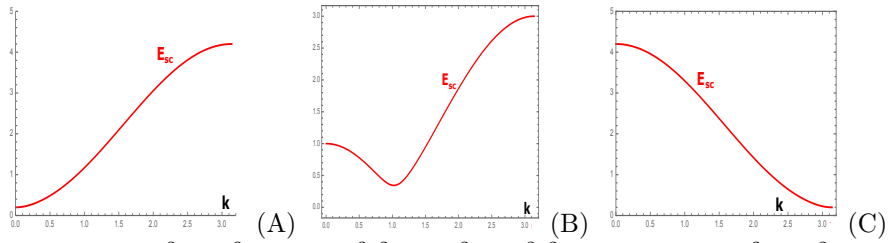
Because of $\cos k^2 \leq 1$, these stationary points exist only in the region of the bulk parameters such that

$$h^2 t^2 \leq 4(t^2 - \Delta_0^2)^2$$

where , of course, also the condition for $E^2 \geq 0$ is satisfied.

The following picture shows the scattering states energy spectrum for some examples of the parameters[1].

- for $\boxed{t^2 - \Delta_0^2 > 0}$, we have



(A) $ht < -2(t^2 - \Delta_0^2)$ (B) $h^2t^2 < 4(t^2 - \Delta_0^2)^2$ (C) $ht > 2(t^2 - \Delta_0^2)$

Figure 4.1: Energy spectrum of Scattering States depending on bulk parameters.

- for $\boxed{t^2 - \Delta_0^2 < 0}$, the roles of $k = 0$ and $k = \pi$ are swapped.

As a final remark, we notice that conditions (a) and (b) are exactly the conditions of reality (2) and (3) that define respectively the edge and the zero modes. This means that the latter two, when existing, originate from scattering states that correspond to minima or maxima of the bulk spectrum. These considerations will be clarified in the next paragraphs.

4.1.2 Edge States

Let us analyze the second condition of reality:

$$\sin k = 0 \quad \Rightarrow \quad k = 0, \pi \quad \Rightarrow \quad z = \pm\lambda \quad \Rightarrow \quad \boxed{z = \pm e^{\eta}} \tag{4.17}$$

where $\eta = \ln \lambda$.

Hence (4.11) becomes:

$$\begin{aligned} E_\eta^2 &= \left[t\left(\pm e^{\eta} \pm e^{-\eta}\right) - h\right]^2 - \Delta_0^2 \left(\pm e^{\eta} \mp e^{-\eta}\right)^2 = \\ &= \left[t\left(\pm 2\cosh\eta\right) - h\right]^2 - \Delta_0^2 \left(\pm 2\sinh\eta\right)^2 = \\ &= \left[2t\cosh\eta \mp h\right]^2 - 4\Delta_0^2 \left(\sinh\eta\right)^2 \end{aligned} \tag{4.18}$$

[1] We are plotting E^2, which is It is the same because we have invariance for $k \to -k$

We have a BCS-like dispersion relation with the hyperbolic function.
For $\eta = 0$, which provides a stationary point for the energy:

$$E_\eta^2\Big|_{\eta=0} = [2t \pm h]^2$$

It obviously coincides with the limit energy of the scattering states; so we can assure that edge states drop from the scattering spectrum at this points.

4.1.3 Zero Modes

The third reality condition is more complicated:

$$\left(t^2 - \Delta_0^2\right) \alpha \cos k - ht = 0$$

Setting $z = \lambda e^{ik} = e^{i(k-i\eta)}$ and recalling that $\alpha = \lambda + \lambda^{-1} = 2\cosh\eta$, this condition gives a relationship between k and η, which, therefore, are not indipendent. Explicitly, we find:

$$\cosh\eta = \frac{ht}{2\left(t^2 - \Delta_0^2\right)\cos k} \tag{4.19}$$

It is also possible to calculate the energy spectrum:

$$E_{k\eta}^2 = \left[2t\cos\left(k - i\eta\right) - h\right]^2 - 4\Delta_0^2(\sin\left(k - i\eta\right))^2 \tag{4.20}$$

Because of $\cosh\eta \geq 1$, proceeding as we have done before for the scattering states, one can show that these solutions exist only in the range of the paramenter:

$$h^2t^2 \geq 2\left(t^2 - \Delta_0^2\right) \tag{4.21}$$

We notice that (4.21) defines the region in which the scattering states develop a minimum at $k \neq 0, \pi$, as shown in figure (B) of (4.1.1).
Combining this with the fact that the value of k, at which such zero modes appears, is exactly the one of the minimum, we can conclude zero modes emerge by dropping out from the scattering spectrum precisely at this minimum.

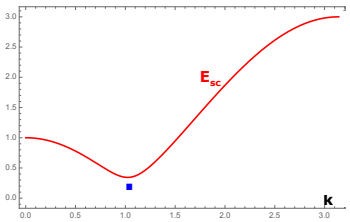


Figure 4.2: An idea of the dropping out of Zero Modes from the scattering spectrum.

A tedious algebraic calculation shows that the energy $E^2_{k\eta}$ is always smaller then the minimum of the scattering band. This means that these modes lie always in the energy band. Therefore, they might reach the zero energy (hence the name zero modes) and become degenerate with the ground state. If it happens, as argued in [14], the system may undergo a quantum phase transition marked by a $\mathbb{Z}_2$ symmetry.

4.2 Boundary conditions

In order to have a hermitian extension of the Hamiltonian, even in the edge, our solutions have to be eigenfunction of $(A+\tilde{B})(A-\tilde{B})$, which is given, considering the boundary parameters, by:

$$\begin{pmatrix}
\mu^2+(t-\Delta_0)^2+(u_A+u_B)^2 & -\mu(t+\Delta_0)-h(t-\Delta_0) & t^2-\Delta_0^2 & \cdot & \cdot & \cdot & 0 & -(u_A+u_B)(t+\Delta_0) & \mu(u_A-u_B)+\nu(u_A+u_B) \\
-\mu(t+\Delta_0)-h(t-\Delta_0) & h^2+2(t^2-\Delta_0^2) & -2ht & 0 & \cdot & \cdot & \cdot & 0 & -(u_A-u_B)(t+\Delta_0) \\
0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \boxed{\text{bulk}} & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\
-(u_A+u_B)(t+\Delta_0) & 0 & \cdot & \cdot & \cdot & \cdot & -2ht & h^2+2(t^2-\Delta_0^2) & -\nu(t-\Delta_0)-h(t+\Delta_0) \\
\mu(u_A-u_B)+\nu(u_A+u_B) & -(u_A-u_B)(t+\Delta_0) & \cdot & \cdot & \cdot & \cdot & t^2-\Delta_0^2 & -\nu(t-\Delta_0)-h(t+\Delta_0) & \nu^2+(t-\Delta_0)^2+(u_A-u_B)^2
\end{pmatrix}$$

It is evident that also the site 1 and the site $N-1$ are influenced by the boundary parameters. In order to simplify a little the calculation, let me use a trick starting from (3.8) and (3.9):

- for $l=0$

$$\begin{aligned}
\Lambda_k g_{k0} &= \sum_i \Big(g_{ki} A_{i0} - \ h_{ki} \tilde{B}_{i0} \Big) \\
\Lambda_k h_{k0} &= \sum_i \Big(- \ h_{ki} A^*_{i0} + \ g_{ki} \tilde{B}_{i0} \Big)
\end{aligned} \tag{4.22}$$

- $l=N$

$$\begin{aligned}
\Lambda_k g_{kN} &= \sum_i \Big(g_{ki} A_{iN} - \ h_{ki} \tilde{B}_{iN} \Big) \\
\Lambda_k h_{kN} &= \sum_i \Big(- \ h_{ki} A^*_{iN} + \ g_{ki} \tilde{B}_{iN} \Big)
\end{aligned} \tag{4.23}$$

Let us start with $i = 0$. Considering only the non vanishing terms of A and the first equation of (4.22) turns in:

$$\begin{aligned}\Lambda_k g_{k0} &= g_{k0}A_{00} + g_{k1}A_{10} + g_{kN}A_{N0} - h_{k1}\tilde{B}_{10} - h_{kN}\tilde{B}_{N0} = \\ &= g_{k0}A_{00} + g_{k1}A_{10} + g_{kN}A_{N0} - h_{k1}\tilde{B}_{10} - h_{kN}\tilde{B}_{N0} + \\ &\quad - h_{k-1}\tilde{B}_{-10} + h_{k-1}\tilde{B}_{-10} + g_{k-1}A_{-10} - g_{k-1}A_{-10}\end{aligned} \tag{4.24}$$

The second one, instead, becomes:

$$\begin{aligned}\Lambda_k h_{k0} &= -h_{k0}A^*_{00} - h_{k1}A^*_{10} - h_{kN}A^*_{N0} + g_{k1}\tilde{B}_{10} + g_{kN}\tilde{B}_{N0} = \\ &= -h_{k0}A^*_{00} - h_{k1}A^*_{10} - h_{kN}A^*_{N0} + g_{k1}\tilde{B}_{10} + g_{kN}\tilde{B}_{N0} + \\ &\quad + g_{k-1}\tilde{B}_{-10} - g_{k-1}\tilde{B}_{-10} - h_{k-1}A^*_{-10} + h_{k-1}A^*_{-10}\end{aligned} \tag{4.25}$$

Working with $i = N$, we obtain:

$$\begin{aligned}\Lambda_k g_{kN} &= g_{k0}A_{0N} + g_{kN-1}A_{N-1N} + g_{kN}A_{NN} - h_{k0}\tilde{B}_{0N} - h_{kN-1}\tilde{B}_{N-1N} = \\ &= g_{k0}A_{0N} + g_{kN-1}A_{N-1N} + g_{kN}A_{NN} - h_{k0}\tilde{B}_{0N} - h_{kN-1}\tilde{B}_{N-1N} + \\ &\quad - h_{kN+1}\tilde{B}_{N+1N} + h_{kN+1}\tilde{B}_{N+1N} + g_{kN+1}A_{N+1N} - g_{kN+1}A_{N+1N}\end{aligned} \tag{4.26}$$

$$\begin{aligned}\Lambda_k h_{kN} &= -h_{k0}A^*_{0N} - h_{kN-1}A^*_{N-1N} - h_{kN}A^*_{NN} + g_{k0}\tilde{B}_{0N} + g_{kN-1}\tilde{B}_{N-1N} = \\ &= -h_{k0}A^*_{0N} - h_{kN-1}A^*_{N-1N} - h_{kN}A^*_{NN} + g_{k0}\tilde{B}_{0N} + g_{kN-1}\tilde{B}_{N-1N} + \\ &\quad + g_{kN+1}\tilde{B}_{N+1N} - g_{kN+1}\tilde{B}_{N+1N} - h_{kN+1}A^*_{N+1N} + h_{kN+1}A^*_{N+1N}\end{aligned} \tag{4.27}$$

Because of the continuity with the bulk solution we have also:

$$\begin{aligned}\Lambda_k g_{k0} &= g_{k0}\bar{A}_{00} + g_{k-1}A_{-10} + g_{k1}A_{10} - h_{k1}\tilde{B}_{10} - h_{k-1}\tilde{B}_{-10} \\ \Lambda_k h_{k0} &= -h_{k0}\bar{A}^*_{00} - h_{k-1}A^*_{-10} - h_{k1}A^*_{10} + g_{k-1}\tilde{B}_{-10} + g_{k1}\tilde{B}_{10}\end{aligned} \tag{4.28}$$

$$\begin{aligned}\Lambda_k g_{kN} &= g_{kN}\bar{A}_{NN} + g_{kN-1}A_{N-1N} + g_{kN+1}A_{N+1N} + \\ &\quad - h_{kN-1}\tilde{B}_{N-1N} - h_{kN+1}\tilde{B}_{N+1N} \\ \Lambda_k h_{kN} &= -h_{kN}\bar{A}^*_{NN} - h_{kN-1}A^*_{N-1N} - h_{kN+1}A^*_{N+1N} + \\ &\quad + g_{kN-1}\tilde{B}_{N-1N} + g_{kN+1}\tilde{B}_{N+1N}\end{aligned} \tag{4.29}$$

Using (4.28) and (4.29) we have to pay attention to $\bar{A}_{00}$ and $\bar{A}_{NN}$; they must represent the bulk chemical potential h, in order to make these last equations true.

Finally, we have:

$$(4.24) \Rightarrow 0 = g_{kN}A_{N0} - h_{kN}\tilde{B}_{N0} + h_{k-1}\tilde{B}_{-10} - g_{k-1}A_{-10} + g_{k0}\left(A_{00} - \bar{A}_{00}\right) = \\ = g_{kN}u_A^* - h_{kN}u_{0_B} + h_{k-1}\Delta_0 + g_{k-1}t + g_{k0}\left(\mu - h\right)$$

$$(4.25) \Rightarrow 0 = -h_{kN}A_{N0}^* + g_{kN}\tilde{B}_{N0} - g_{k-1}\tilde{B}_{-10} + h_{k-1}A_{-10}^* - h_{k0}\left(A_{00} - \bar{A}_{00}\right) = \\ = -h_{kN}u_A + g_{kN}u_{0_B} - g_{k-1}\Delta_0 - h_{k-1}t - h_{k0}\left(\mu - h\right)$$

$$(4.26) \Rightarrow 0 = g_{k0}A_{0N} - h_{k0}\tilde{B}_{0N} + h_{kN+1}\tilde{B}_{N+1N} - g_{kN+1}A_{N+1N} + g_{kN}\left(A_{NN} - \bar{A}_{NN}\right) = \\ = g_{k0}u_A + h_{k0}u_{0_B} - h_{kN+1}\Delta_0 + g_{kN+1}t + g_{kN}\left(\nu - h\right)$$

$$(4.27) \Rightarrow 0 = -h_{k0}A_{0N}^* - h_{kN}\left(A_{NN}^* - \bar{A}_{NN}\right) + g_{k0}\tilde{B}_{0N} - g_{kN+1}\tilde{B}_{N+1N} + h_{kN+1}A_{N+1N}^* = \\ = -h_{k0}u_A^* - g_{k0}u_{0_B} + g_{kN+1}\Delta_0 - h_{kN+1}t - h_{kN}\left(\nu - h\right)$$

Simplifying these expressions and considering the elements of the matrices **A** and **B**, we get

$$\begin{aligned} g_{kN}u_A^* - h_{kN}u_{0_B} + h_{k-1}\Delta_0 + g_{k-1}t + g_{k0}\left(\mu - h\right) &= 0 \\ -h_{kN}u_A + g_{kN}u_{0_B} - g_{k-1}\Delta_0 - h_{k-1}t - h_{k0}\left(\mu - h\right) &= 0 \\ g_{k0}u_A + h_{k0}u_{0_B} - h_{k\ N+1}\Delta_0 + g_{kN+1}t + g_{kN}\left(\nu - h\right) &= 0 \\ -h_{k0}u_A^* - g_{k0}u_{0_B} + g_{k\ N+1}\Delta_0 - h_{kN+1}t - h_{kN}\left(\nu - h\right) &= 0 \end{aligned} \tag{4.30}$$

Consider the following general ansatz of solution, which, up to a redefinition of the coefficient is equivalent to (4.9):

$$\begin{aligned} g_{ml} &= a_m z^l + b_m z^{N-l} \\ h_{ml} &= c_m z^l + d_m z^{N-l} \end{aligned} \tag{4.31}$$

For scattering states with $z = e^{ik}$, equations (4.30) fixes the discrete values of k of the band which are compatible with boundary conditions. Such an ansatz can be considered for edge states, too; in the limit of large L, for edge states such that $z^j = z^{-\alpha j}$,with $\alpha > 0$, it is possible to make the following approximation:

$$\begin{array}{cc} g_{m-1} \sim az^{-1} & h_{m-1} \sim cz^{-1} \\ g_{m0} \sim a & h_{m0} \sim c \\ g_{mN} \sim b & h_{mN} \sim d \\ g_{mN-1} \sim bz^{-1} & h_{mN-1} \sim dz^{-1} \end{array}$$

considering that $z^{-\alpha j} \xrightarrow{j\ large} 0$ and $z^{-\alpha(N-j)} \xrightarrow{j\ small} 0$.
Thus, equations (4.30) become

$$\begin{aligned} bu_A^* - du_{0_B} + cz^{-1}\Delta_0 + az^{-1}t + a(\mu - h) = 0 \\ -du_A + bu_{0_B} - az^{-1}\Delta_0 - cz^{-1}t - c(\mu - h) = 0 \\ au_A + cu_{0_B} - dz^{-1}\Delta_0 + bz^{-1}t + b(\nu - h) = 0 \\ -cu_A^* - au_{0_B} + bz^{-1}\Delta_0 - dz^{-1}t - d(\nu - h) = 0 \end{aligned}$$

This system has non-trivial solution for (a, b, c, d), only if

$$D = \begin{pmatrix} tz^{-1} + (\mu - h) & u_A^* & \Delta_0 z^{-1} & -u_B \\ -\Delta_0 z^{-1} & u_B & -tz^{-1} - (\mu - h) & -u_A \\ u_A & tz^{-1} + (\nu - h) & u_B & -\Delta_0 z^{-1} \\ -u_B & \Delta_0^{-1} & -u_A^* & -tz^{-1} - (\nu - h) \end{pmatrix}$$

has null determinant.
Imposing this condition, a fourth order equation of z^{-1} is obtained, that gives four solutions, depending on the parameter at the edge.
Now, as illustrated in the previous chapter, the combinations that diagonalize the Hamiltonian are given by $(a \pm c)$ and $(b \pm d)$ or alternatively by $(a \pm b)$ and $(c \mp d)$; therefore, the action of the Hamiltonian can be reduced to a 2x2 matrix. The same combinations must be eigenfunctions for the edge sites. The reduction[2] yields a second order equation for z^{-1} . In fact, choosing the combinations $(a \pm b)$ and $(c \mp d)$, we get to:

$$\begin{pmatrix} (t - \Delta_0)z^{-1} + (\mu - h) & u_A + u_B \\ u_B - u_A* & -(\Delta_0 + t)z^{-1} - (\nu - h) \end{pmatrix} \begin{pmatrix} a \pm b \\ c \mp d \end{pmatrix} = 0$$

which again has non-trivial solutions only if :

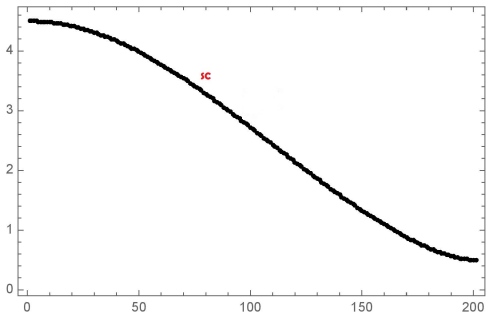
$$(t^2 - \Delta_0^2)z^{-2} + (-2th + t(\mu + \nu) + \Delta_0(\mu - \nu))z^{-1} + \mu\nu + h^2 - h(\mu + \nu) + u_B^2 - |u_A|^2 = 0 \quad (4.32)$$

A similar procedure can be carried out for zero modes, thus finding all possible eigenvalues of tha Hamiltonian with specified boundary conditions.

Summing up, in this chapter we have shown how the Lieb-Shultz-Mattis technique can be analitically implemented after using an ansatz for the wave function of the type (4.31)[3] and exactly imposing boundary conditions.

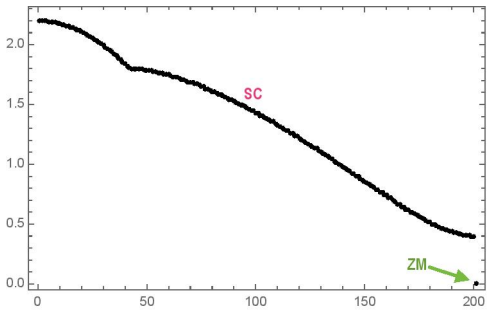
[2] Actually this reduction is symply given by the symmetry $t \to -t$ and $\Delta_0 \to -\Delta_0$
[3] Incidentally we remark that such an ansatz is what is known as *Bethe Ansatz* [7]

LSM method is also easily implemented numerically via a Mathematica code. As a summary of results, we show below the energy spectrum of the Hamiltonian $(A+\tilde{B})(A-\tilde{B})$. for different values of the boundary parameters[4].



When the chain is truncated at the edge, for small edge chemical potentials, no edge neither zero modes appear, in complete analogy with the free case.

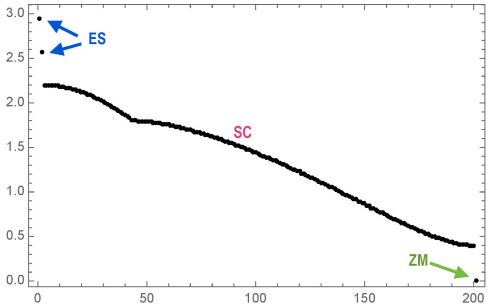
Figure 4.3: $t = 1$; $\Delta = 0.2$; $h = \mu = \nu = -0.2$; $u_A = u_B = 0.0$.



As in the free case, for not too large μ and ν, no edge state is present. However interactions open up a gap in which zero modes might appear.

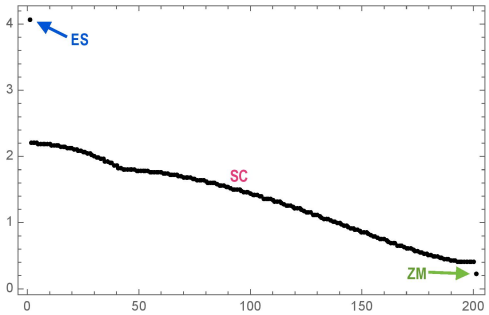
Figure 4.4: $t = 1$; $\Delta = 0.2$; $h = 0.2$; $\mu = \nu = -2.0$; $u_A = u_B = 0.0$.

[4]The energies are ordered in aa decreasing way.



Even if u_A is zero, for strong enough μ and ν, edge states can appear simultaneously with zero modes.

Figure 4.5: $t = 1$; $\Delta = 0.2$; $h = 0.2$; $\mu = -2.0$; $\nu = -2.5$; $u_A = u_B = 0.0$



When u_A is turned on, a probability current is established between the two edges and the energy of the zero modes increases until they fall again into the scattering spectrum.

Figure 4.6: $t = 1$; $\Delta = 0.2$; $h = 0.2$; $\mu = -2.0$; $\nu = -2,5$; $u_A = 1.5$; $u_B = 0.0$

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Conclusions and Outlooks

The possibility of manipulating boundary conditions in a controlled way on a lattice paves the way for an accurate investigation of edge properties.
The study of a fermionic Hamiltonian with the most general boundary conditions has been carried on in a 1-D chain with lattice step $a = 1$. For free spinless fermions, two kinds of edge states are possible: uniform edge states that emerge from the bulk spectrum at $k = 0$ and staggered edge states which drop out at $k = \pi$.
In the continuum limit, edge states are bound eigenfunctions at one or the other boundary point of the chain depending on the chemical potentials chosen for such boundaries. When there is no hopping between the ending sites, the two edge states are indipendent; turning on a probability current flux, instead, they are no longer extraneous and they can fall again into the scattering spectrum.
In the presence of a BCS-like interaction, simultaneously with the emerging of edge states, the system can afford the arising of another kind of states, the so-called *zero modes*; the existence of these new modes is determined both by bulk and edge parameters.
While edge states show energies larger than the scattering spectrum, zero modes energies belong to the gap generated by the interaction; it follows that edge modes can become degenerate with the ground state providing a new quantum phase.

The procedure followed in a 1-D chain can be extended to a two-dimensional lattice, starting from the description of free fermions through an Hamiltonian of this form:

$$H_{free} = \sum_i \sum_j \left[-t_i \left(\hat{c}^\dagger_{i+1,j} \hat{c}_{i,j} + h.c. \right) - t_j \left(\hat{c}^\dagger_{i,j+1} \hat{c}_{i,j} + h.c. \right) \right] + h_{i,j} \hat{c}^\dagger_{i,j} \hat{c}_{i,j} \tag{4.33}$$

where $\hat{c}_{i,j}$, $\hat{c}^\dagger_{i,j}$ are fermionic annihilation and creation operators. The first term describes the dynamics along one direction, that we label by $\hat{x}$, while the second term provides the hopping along the other, i.e. $\hat{y}$; the third term represents a chemical potential at each site. As long as we are describing free fermions an ansatz with indipendent solutions for the $\hat{x}$ and $\hat{y}$ directions is acceptable and implementing boundary conditions could be quite simple.
However, if we consider some interactions, for example with an external magnetic field,

several problems arise.
On the other side, the action of a magnetic field can be treated by considering that the fermions acquire a phase each time they jump from one site to the other. It is just the Ahranov-Bohm effect in a discrete lattice. Then, if it is possible to perform a local U(1) transformation on each site[1], such that we have a uniform complex hopping parameter per direction, we will able to diagonalize the Hamiltonian through the extended Lieb-Shultz-Mattis technique and to implement boundary conditions.
Such a mathematical description can be useful to investigate lot of new topics of research interest. For instance, it could explain chiral edge states in a 1-D fermionic Hamiltonian, where a syntethic dimension is given endowing each site with M internal states, as it has been observed in recent experiments[9]. Otherwise, it can be useful also to implement a simulation of quantum field theories; in fact, using ultracold atoms, fermionic systems share qualitative features with QCD, including chiral symmetry breaking and restoration at non-zero temperature[5].

Appendix A

Self-Adjoint Extension of Unbounded Operators: Deficiency Indices

Let T be an unbounded linear operator on a Hilbert space $\mathcal{H}$ such that its domain $D(T)$ is dense in $\mathcal{H}$.
Namely

$$D(T)^{-} = \mathcal{H} \quad \Rightarrow \quad D(T)^{\perp} = 0 \tag{A.1}$$

Let me recall first some definition and theorems of linear operators in order to understand the Cayley transform[1].

Def. $T : D(T) \to \mathcal{H}$ is symmetric if $\langle \phi | T\psi \rangle = \langle T\phi | \psi \rangle \quad \forall \psi,\ \phi \in D(T)$

Th. $T^{\dagger}$ is univocally defined as adjoint operator of T only if $D(T)^{-} = \mathcal{H}$ and it satisfies

$$\langle \phi | T\psi \rangle = \left\langle T^{\dagger}\phi | \psi \right\rangle \quad \forall \psi \in D(T), \phi \in D(T^{\dagger}) \tag{A.2}$$

Th. *Fisher-Reisz for linear functionals.*
$\forall$ linear continuous functional $f \in \mathcal{H}^{*}\ \exists!\ x\ \in \mathcal{H} | f(y) = \langle x | y \rangle \quad \forall y \in \mathcal{H}$

Th. *Fisher-Reisz for sesquilinear functionals.*
Let $\omega : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ be a sesquilinear continuous functional. Then

$$\forall y \in \mathcal{H} \ \text{ fixed } \quad \exists!\ \ \theta_y \text{ such that } \ \omega(x, y) = \langle x | \theta_y \rangle \, .$$

[1] I will not prove any theorem because it is out of my purpose. They can be find in ?????

Then a linear application $T : \mathcal{H} \to \mathcal{H}$ is defined. Namely:

$$\theta_y = Ty \quad \Rightarrow \quad \omega(x,y) = \langle x|Ty\rangle$$
$$\Rightarrow ||T|| = ||\omega||$$

Fisher-Reisz' theorem can be applied only if the functional is continuous. That is the reason why it is necessary to pay attention to the domain of definition of $T^\dagger$. Explicitly: $\forall\ \phi\ \in\ \mathcal{H} : \phi\ \to\ \langle\phi|T\psi\rangle$ is a linear functional, but it is not continuous.
So let's define:

$$D^* = \{\psi \in \mathcal{H}\ ,\ |\ \langle\phi|T\psi\rangle\ | \leq C_\psi ||\psi||\}$$

Hence, the functional is bounded - so, continuous - $\forall\ \psi \in D^*$.
At this point, thanks to *Fisher-Reisz*' theorem $\exists!\ \phi^*$ such that $\langle\phi|T\psi\rangle = \langle\phi^*|\psi\rangle$ and $\psi^* = T^\dagger\psi$.
The uniqueness is garanteed by the property $D(T)^\perp = 0$.
In fact, if $\exists\ \phi^*,\ \phi^{**}$ such that $\langle\phi|T\psi\rangle = \langle\phi^*|\psi\rangle = \langle\phi^{**}|T\psi\rangle$ then

$$\langle(\phi^* - \phi^{**})|T\psi\rangle = 0 \quad \Rightarrow \quad (\phi^* - \phi^{**})\ \perp\ \psi$$

$$D(T)^\perp = 0 \quad \Rightarrow \quad (\phi^* - \phi^{**}) = 0 \quad \Rightarrow \quad \phi^* = \phi^{**}$$

. So it can be provided a new definition of symmetric operator:

Def. *Symmetric Operator*
Let $T : D(T) \to \mathcal{H}$ be a linear operator. $D(T)^- = \mathcal{H}$.
Then T is symmetric only if

$$T = T^\dagger\big|_{D(T)}$$

Hence, the adjoint of a symmetric operator is an extension of it.

Def. *Self-Adjoint Operator*
Let $T : D(T) \to \mathcal{H}$ be a linear symmetric operator. $D(T)^- = \mathcal{H}$.
Then T is self-adjoint if

$$D(T) = D(T^\dagger) \quad \Rightarrow \quad T = T^\dagger$$

Def. *Graphic of an Operator*

$$\mathcal{G}(T) = \{(x,y) \in \mathcal{H} \oplus \mathcal{H}|\ y = Tx,\ x \in D(T)\}$$

Given $\Pi_1 : \mathcal{H} \oplus \mathcal{H} \to \mathcal{H}$ such that $\Pi_1(x,y) = x$

$$\mathcal{G}(T)\ \text{ graphic of T} \quad \Leftrightarrow\ \mathcal{N}(\Pi_1\big|_{\mathcal{G}(A)}) = \{(0,0)\} \tag{A.3}$$

where $\mathcal{N}$ is the kernel. Namely $\mathcal{N}(\Pi_1) = \{(x,y)|\Pi_1(x,y) = 0\}$.

Def. *Closed Operator*
Let $T : D(T) \to \mathcal{H}$ be a linear operator.
T is closed if $\forall x_n \in D(T)$ such that

$$\left.\begin{array}{c} \exists \lim\limits_{n\to\infty} x_n = x \\ \exists \lim\limits_{n\to\infty} Tx_n = y \end{array}\right\} \quad \Rightarrow \quad y = Tx$$

It is similar to the property of continuity, in which however the existence of $\lim\limits_{n\to\infty} Ax_n$ is implicit.

Th. *Closed Operator*
Let $T : D(T) \to \mathcal{H}$ be a linear operator.
T is closed if its graphic is closed.

$$\mathcal{G}(T)^- = \mathcal{G}(T) \quad \Leftrightarrow \quad T \quad \text{is closed}$$

The closure of $\mathcal{G}(A)$ guarantees the completeness; so $\mathcal{G}(A)$ is an Hilbert space, endowed with the T-scalar product:

$$\langle (x, Tx), (x', Tx') \rangle = \langle x, x' \rangle + \langle Tx, Tx' \rangle$$

where the scalar products of the r.h.s. are given by the standard scalar product in $\mathcal{H}$.

Def. *Closable Operator*
Let $T : D(T) \to \mathcal{H}$ be a linear operator. Then T is closable if $\mathcal{G}(T)^-$ is the graphic of an operator T^-. Then T^- is the closure of T.

Th. *Graphic of the Adjoint Operator*
Let $T : D(T) \to \mathcal{H}$ be a linear operator. Let $\tau : \mathcal{G}(T) \to \mathcal{H}$ such that $\tau(x, y) = (-y, x)$, where $y = Tx$. Then,

$$D(T)^- = \mathcal{H} \quad \Leftrightarrow \quad [\tau\left(\mathcal{G}(T)\right)]^\perp = \mathcal{G}(T^\dagger)$$

The adjoint operator of T exists if and only if the orthogonal complement of $[\tau(\mathcal{G}(T))]^\perp$ is the graphic of an operator, namely it satisfies (A.3). This operator is exactly the adjoint one of T.
Now, $[\tau(\mathcal{G}(T))]^\perp$, being an orthoganal complement, is a closed subspace and it is the graphic of a closed operator that is $T^\dagger$.

Th. *Essentially Self-Adjoint operator*
Let $T : D(T) \to \mathcal{H}$ be a linear operator.
T is essentialy self-adjoint if $D(T)^- = \mathcal{H}$, it is closable and $D(T^\dagger)^- = \mathcal{H}$

Dim: T closable $\Rightarrow \quad [\mathcal{G}(T)]^- = \mathcal{G}(T^-)$.
$D(T)^- = \mathcal{H} \quad \Rightarrow \quad \exists\, T^\dagger$.
$D(T^\dagger)^- = \mathcal{H} \quad \Rightarrow \quad \exists\, (T^\dagger)^\dagger$.
Then $[\tau(\mathcal{G}(T))]^\perp = \mathcal{G}(T^\dagger)$ and $\left[\tau\left[\tau(\mathcal{G}(T))\right]^\perp\right]^\perp = \mathcal{G}((T^\dagger)^\dagger)$.
However

$$\left[\tau\left[\tau(\mathcal{G}(T))\right]^\perp\right]^\perp = \left[[\mathcal{G}(T)]^\perp\right]^\perp = \mathcal{G}((T^-)$$
$$\Rightarrow\ \mathcal{G}((T^\dagger)^\dagger) = \mathcal{G}((T^-) \Rightarrow \quad (T^\dagger)^\dagger = T^-$$

Th. *Self-Adjoint Operator*
Let $T : D(T) \to \mathcal{H}$ be a linear symmetric operator. $D(T)^- = \mathcal{H}$.
The following statements are equivalent:

(a) T is self-adjoint : $D(T) = D(T^\dagger)$;

(b) T is closed and $\mathcal{N}(T^\dagger \pm i\mathbb{I}) = \{0\}$;

(c) $\mathcal{R}(T \pm i\mathbb{I}) = \mathcal{H}$, the range of $(T \pm i\mathbb{I})$ is closed.

Th. *Essentially Self-Adjoint Operator*
Let $T : D(T) \to \mathcal{H}$ be a linear symmetric operator. $D(T)^- = \mathcal{H}$.
The following statements are equivalent:

(a) T is essentially self-adjoint;

(b) $\mathcal{N}(T^\dagger \pm i\mathbb{I}) = \{0\}$;

(c) $\mathcal{R}(T \pm i\mathbb{I})^- = \mathcal{H}$.

After this overview, it is possible to introduce the Cayley transform.

Th. *Cayley Transform*
Let $\mathcal{H}$ be an Hilbert space and $T : D(T) \subseteq \mathcal{H} \to \mathcal{H}$ be a symmetric linear operator. Then

$$V := (T + i\mathbb{I})(T - i\mathbb{I})^{-1} \qquad \textit{Cayley Transform of } T \tag{A.4}$$

is a surjective isometry $V : \mathcal{R}(T - i\mathbb{I}) \to \mathcal{R}(T + i\mathbb{I})$ and are valid:

(a) $D(T) = \mathcal{R}(\mathbb{I} - V)$;

(b) $T = -i(\mathbb{I} + V)(\mathbb{I} - V)^{-1}$;

(c) T is self-adjoint if and only if V is a unitary operator on $\mathcal{H}$;

(d) Given a unitary operator $V : \mathcal{H} \to \mathcal{H}$, if $(\mathbb{I} - V)$ is injective, then it is the Caley transform of a symmetric operator T defined as in (a).

Def. *Deficiency indices*
Let $T : D(T) \to \mathcal{H}$ be a linear symmetric operator. Its *deficiency indeces* are defined as:

$$d_{\pm}(T) = dim(\mathcal{N}(T^{\dagger} \pm i\mathbb{I}))$$

The *deficiency indices* indicate in some way how much the operator is not self-adjoint. In fact, as mentioned before:

- T is closed and $\mathcal{N}(T^{\dagger} \pm i\mathbb{I}) = \{0\} \Leftrightarrow T$ is self-adjoint;
- $\mathcal{N}(T^{\dagger} \pm i\mathbb{I}) = \{0\} \Leftrightarrow T$ is essentially self-adjoint.

Th. *Deficiency indices*
Let $T : D(T) \to \mathcal{H}$ be a linear symmetric operator. Then

(a) T admits self-adjoint extensions if and only if $d_+(T) = d_-(T)$;

(b) If $d_+(T) = d_-(T)$ then $\exists$ a bijective correspondence between the self-adjoint extensions of T an the surjective isometries defined before. More precisely, T admits many self-adjoint extensions how many are the surjective isometries.
Let me remember that $\mathcal{N}(T^{\dagger} \pm i\mathbb{I}) = [\mathcal{R}(T \mp i\mathbb{I})]^{\perp}$. If $dim(\mathcal{N}(T^{\dagger} \pm i\mathbb{I}) = 0$, then $[\mathcal{R}(T \mp i\mathbb{I})]^{-} = \mathcal{H}$ and $V := (T + i\mathbb{I})(T - i\mathbb{I})^{-1}$ is unitary[2] and the only Cayley transform. In fact if T is essentially self-adjoint, it admits only one self-adjoint extension(its closure):

$$T^{-} = -i(\mathbb{I} + V)(\mathbb{I} - V)^{-1}$$

where V is a unitary operator.

Let me conclude giving an idea of how a self-adjoint extension can be built. Given a linear symmetric operator $T : D(T) \to \mathcal{H}$, such that $d_+(T) = d_-(T)$, its Cayley transform:

$$U = (T + i\mathbb{I})(T - i\mathbb{I})^{-1}$$

is an isometry $U : \mathcal{R}(T - i\mathbb{I}) \to \mathcal{R}(T + i\mathbb{I})$. It is bounded, so it can be extended to the closures of these two spaces.
Because of $d_+(T) = d_-(T)$, $\exists$ another isometry $U_0 : \mathcal{N}(T^{\dagger} + i\mathbb{I}) \to \mathcal{N}(T^{\dagger} - i\mathbb{I})$. Then:

$$W = U \otimes U_0 : [\mathcal{R}(T - i\mathbb{I})]^{-} \oplus \mathcal{N}(T^{\dagger} + i\mathbb{I}) \quad \to \quad [\mathcal{R}(T + i\mathbb{I})]^{-} \oplus \mathcal{N}(T^{\dagger} - i\mathbb{I})$$
$$W : \mathcal{H} \ \to \mathcal{H}$$

[2] An isomtery becomes a unitary operator if its domain is all $\mathcal{H}$

Therefore W, as a unitary operator, is the Cayley transform of a self-adjoint operator $\tilde{T}$, that is an extension of T. For all extensions what changes is U_0. If it exists is possible to create a self-adjoint extension.

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