## Utrecht University

Institute for Theoretical Physics

Master's Thesis

# Conductance in Sierpinski Carpets on a Hofstadter Model 

Author:
Michał van Hooft, BSc

Supervisor:
Dr. Lars Fritz

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## Chapter 1

## Introduction

### 1.1 Motivation

During recent years the study of topological insulators has grown to an active field in condensed matter physics. Topological insulators are materials where the bulk of the system is insulating, but where there are conducting states at the edge of the material, we illustrate this situation in figure 1.1.


Figure 1.1: Sketch of a topological insulator. Taken from [1].
Through the classifying system known as the 'ten-fold way' one may know in advance what types of topological invariants are allowed in a system. The 'ten-fold way' classifies models based on their symmetries. One obtains ten categories by classifying a system by three symmetries: time-reversal, particle-hole and chiral symmetry. For each of these categories the dimension then influences the topological invariants allowed [2].

However, there are systems in nature that do not fall in any of these categories. For example fractals, which have a non-integer dimension. So what happens to the topological invariants in a fractal object? To investigate this we study the chiral modes in a Hofstadter model, where we create a lattice shaped as a Sierpinski carpet. We study the chiral modes, because in a Hofstadter model they relate directly to the topological invariant, the first Chern number [3].

Additionally, to investigating chiral edge modes, the study of conductance on a fractal is interesting in its own right, as it is known that the density of states in fractals have a fractal distribution. Literature on the similar systems shows that fractal properties may also be observed in the wave-functions and the bulk
conductance $[4,5,6]$.
Furthermore, fractal structures have unique properties that put them outside of typical descriptions. The Sierpinski carpet, for example, has no translational invariance or a clear separation into edge and bulk regions. Such properties mean that typical descriptions for describing transport do not apply. Yet a domain that falls outside of the scope of standard description, also allows for the discovery of new phenomena.

Fractals are not only of theoretical interest, but can actually be created in the laboratory [4]. In this thesis we implement the Sierpinski carpet by starting with a tight-binding model on a square lattice and removing atoms corresponding to the holes of the Sierpinski carpet. This we display in figure 1.2.


Figure 1.2: The implementation of the Sierpinski carpet into the tight-binding model.
One might be mistaken that constructing such a structure on the atomic scale is impossible, but such manipulations can be performed through the use of scanning tunnelling microscopy [7]. Scanning tunnelling microscopes can image surfaces on the atomic level. They do this by putting a needle close to the surface and measuring the quantum tunnelling to the surface. Yet the same instrument may be used to pick up atoms and place them at a desired spot. A well known example of this is that IBM made their logo on the atomic scale by placing 35 xenon atoms on a crystal of nickel. Through the use of such techniques one may also create a Sierpinski carpet. In fact, the same techniques have already been used to create a Sierpinski triangle [4].

### 1.2 Outline

Chapter 2 begins a brief introduction to fractals and fractal dimension. Then we introduce the tight-binding model and how it derives from continuum models. This derivation is done for two different continuum models. The first continuum model is the free-electron model. It has limited applicability to our system, yet it is useful for making a connection between the integer quantum Hall effect and the Hofstadter model, which we will use later. The second continuum model assumes that the lattice potential causes the wave functions to be localized at the lattice sites. The last part of chapter 2 focuses on the integer quantum Hall effect. The integer quantum Hall effect provides a good introduction to the Landau levels and chiral edge modes, that are the focus of this thesis.

Chapter 3 focusses on the method used to calculate the conductance in a tight-binding model. We begin this chapter with the Landauer-Büttiker formalism, which allows us to relate the conductance to the transmission. The transmission in turn depends on Green's functions. As such we explain both concepts and how they relate to each other. The calculation of the Green's functions is made using the recursive Green's function equations. We derive these equations and show how they are used to calculate the conductance.

In chapter 4 we consider simple wires and the Hofstadter model. This allows us to become familiar with
numerical results, as we know from literature how the system should behave. We begin with investigating a perfect wire and the effects of impurities on this wire. We then introduce a magnetic field into the model giving us the Hofstadter model with an edge [8]. Due to this edge in our system we observe chiral edge modes.

Chapter 5 is devoted to the numerical results of the Sierpinski carpet. To gain additional understanding of the system we also look at the resistance to impurities, scaling and the wave-function localization. We find that there are 4 categories of states. In figure 1.3 we show examples of these states. The first category contains states that are localized inside the fractal. The transmission in these regions shows fluctuation that most likely have a fractal distribution. The second category has states that are localized on the edge and is resistant to impurities, these are chiral edge modes. We also find a category of states that is not stable to impurities, but remains identical under scaling and these are also localized on the edge. Thus these modes have no chirality. The last type of state are states that form a large square structure and where the transmission is not stable to noise, but does remain identical under scaling.


Figure 1.3: Examples of the localization of different states in the Sierpinski carpet.

Readers who are mainly interested in the results are recommended to take a quick look at the Hoffstadter results of chapter 4 and then continue to chapter 5.

## Chapter 2

## Theoretical Background

### 2.1 Introduction to Fractals

Fractals are objects with a non-integer dimension. A wide range of physical phenomena show fractal behaviour, as they show up in a wide range of physical phenomena such as electric discharges or in the description of polymers, to subjects in biology and geographical features. We will explain in this section what it means for an object to be a fractal, by explaining how they relate to two concepts: self-similarity and a generalised dimension based on scaling.

We begin with introducing the concept of self-similarity in fractals. Many fractals are specified through a recursive procedure that performs a manipulation and then divides the system into smaller components that undergo the same recursive procedure. This procedure is then repeated to infinity. Such an object has self-similarity by virtue of the recursive procedure. An example of this is the Koch curve is shown in figure 2.1. To generate a Koch curve one starts with a line, cuts this line in three pieces, replaces the middle piece with two lines that extent outward and this procedure is repeated for all four new lines. This procedure is then repeated infinitely often to obtain the Koch curve.


Figure 2.1: The recursive procedure that generates the Koch curve, where $n$ is the number of times the recursive procedure was applied. The Koch curve has fractal dimension $d_{H}=\log (4) / \log (3) \approx 1.26$. This image was taken from [9].

The self-similarity of deterministic fractals such as the Koch curve is easy to quantify. However, even though many objects are not made in a deterministic fashion, they appear self-similar to the human eye. We show
one such example in figure 2.2.


Figure 2.2: Electrodeposition of copper. The right panel is a magnification of the red box in the right panel. This image was taken from [10].

To describe non-deterministic fractals we introduce a generalised dimension. We base this generalised dimension on the scaling of an object. For example the line, square and cube are examples of objects that are one, two and three-dimensional. If we scale these objects by doubling the length in each direction of these objects, we find that what we could call a volume for these objects, increases by $2^{1}, 2^{2}$ and $2^{3}$. Thus we find that the dimension of an object relates to the power of the scaling.

One way of defining a generalised dimension is through the box-counting dimension. In the box-counting dimension we change the resolution we use to look at an object, instead of scaling the object. These two concepts are related as by changing the resolution we use to look at the object, we scale the space where the object lives in. For the box-counting dimension one constructs a mesh with spacings of length $l$. One then counts the amount of boxes, $N(l)$, of this mesh which contain a part of the object. The dimension of the object is then found by the limit of $l$ to zero,

$$
\begin{equation*}
d_{\mathrm{box}}=\lim _{l \rightarrow 0} \frac{\log (N(l))}{-\log (l)} \tag{2.1}
\end{equation*}
$$

This definition ensures that objects that are clearly of a specific integer dimension have this dimension. For example the line, where $N(l) \approx 1 / l$, is then one-dimensional. Other objects such as the Koch curve have a scaling where $N(l) \approx(1 / l)^{4 / 3}$, thus its dimension is fractal.

When describing physical systems fractal structures do not continue forever, because at the very least we have a natural cut-off once we reach atomic scale. In the mathematical definition of a fractal this implies the object is not strictly a fractal. However, self-similar behaviour may still be observed across multiple length scales, thus the object has fractal character. We quantify this character by calculating the box dimension for a fixed $l$ and if this is constant across multiple orders of the length, then we call this system a fractal.

To illustrate this concept we consider the coastline of Great Britain. Applying the box counting algorithm yields a dimension of $d_{\text {box }} \approx 1.25$ [11], as is shown in figure 2.3.

In this section we introduced fractals by the box-counting dimension. We chose this option as it is the most intuitive to explain, but generally the Hausdorf dimension is used to classify objects. However, except for specific counter examples, that are not considered in this thesis, the box dimension and Hausdorff dimension coincide [13].


Figure 2.3: The box counting method to find $N(l)$ applied to the coastline of Great Britain. This image was taken from [12].

### 2.2 Tight-Binding Model

All research done in this thesis can on a microscopical level be written as a tight-binding model. A notable exception to this is the derivation of the Hall effect.

The tight-binding models is defined in terms of second quantization, where we consider two types of operators: the creation operator, $\hat{c}_{i}^{\dagger}$, and the annihilation operator, $\hat{c}_{i}$. In this thesis the operators are labelled by the index $i$. In general may contain a multitude of quantum numbers, i.e. spins momenta or orbitals, but in this thesis we restrict ourselves to lattice sites.
Further, here $\hat{c}_{i}^{\dagger}$ and $\hat{c}_{i}$ are always fermionic operators and thus have the anti-commutation relations $\left\{\hat{c}_{i}^{\dagger}, \hat{c}_{j}\right\}=\delta_{i, j}$ and $\left\{\hat{c}_{i}^{\dagger}, \hat{c}_{j}^{\dagger}\right\}=\left\{\hat{c}_{i}, \hat{c}_{j}\right\}=0$.
The interpretation of $\hat{c}_{i}^{\dagger}$ is that it creates an electron at site $i$ and that $\hat{c}_{i}$ removes an electron. We will more formally derive this connection in section 2.3.2.
In the scope of this thesis the the tight-binding model describes electrons localized on a lattice of atoms. This lattice generates a strong potential, $V(x)$, where the minima are located on the atoms. This potential causes the wave-functions, $\psi(x)$, to be strongly localised near the minima of the potential, as illustrated in figure 2.4.


Figure 2.4: Top: the localized wave-functions. Middle: The potential induced by the lattice. Bottom: The lattice of atoms.

### 2.2.1 One-Dimensional Wire

One of the most simple models we may write down for the tight-binding model is that of a perfect onedimensional wire with only nearest neighbour hopping,

$$
\begin{equation*}
\hat{H}=\sum_{i} \mu \hat{c}_{i}^{\dagger} \hat{c}_{i}+t \hat{c}_{i}^{\dagger} \hat{c}_{i+1}+t \hat{c}_{i+1}^{\dagger} \hat{c}_{i} \tag{2.2}
\end{equation*}
$$

This simplistic model already contains most important ingredients used in this thesis. The $\mu \hat{c}_{i}^{\dagger} \hat{c}_{i}$ term represents the energy of an electron bound to a single site, commonly referred to as global chemical potential. In some models we make the chemical potential dependant on the site, $\mu_{i}$. In these models we refer to $\mu_{i}$ as the local chemical potential.

The $t \hat{c}_{i}^{\dagger} \hat{c}_{i+1}$ term represent an electron disappearing from site $i$ and appearing at site $i+1 . t \hat{c}_{i+1}^{\dagger} \hat{c}_{i}$ describes the opposite process. The terms proportional to $t$ are referred to as the hopping terms.
The solutions to the Schrödinger equation with the Hamiltonian of equation (2.2) are superpositions of creation operators in the form of $\Psi=\sum_{j} b_{j} \hat{c}_{j}^{\dagger}|0\rangle$. Solving the Schrödinger equation for $E$ yields

$$
\begin{equation*}
E b_{j}=t b_{j+1}+\mu b_{j}+t b_{j-1} \tag{2.3}
\end{equation*}
$$

Due to translational invariance, the solutions of this equation are plane waves, $b_{j}=\exp (i k j)$, where $k$ is a dimensionless momentum,

$$
\begin{equation*}
E e^{i k j}=t e^{i k(j+1)}+\mu e^{i k j}+t e^{i k(j-1)} \tag{2.4}
\end{equation*}
$$

We divide by $e^{i k j}$ and solve for $E$ to obtain the spectrum of the one-dimensional wire

$$
\begin{align*}
E & =\mu+t\left(e^{i k}+e^{-i k}\right)  \tag{2.5}\\
& =\mu+2 t \cos (k) \tag{2.6}
\end{align*}
$$

The two dimensional generalisation of this model, where the lattice has a square structure, is solved by plane wave in both directions. The energies of this model are $E=\mu+2 t \cos \left(k_{x}\right)+2 t \cos \left(k_{y}\right)$.

### 2.2.2 General Models

In this thesis we describe many different tight-binding models, but all these models may be expressed as

$$
\begin{equation*}
\hat{H}=\sum_{i, j} \hat{c}_{i}^{\dagger} \mathbf{H}_{i, j} \hat{c}_{j} . \tag{2.7}
\end{equation*}
$$

$\mathbf{H}$ is a hermitian matrix that containing all information of the system. The diagonal entries refer to the local chemical potentials, $\mathbf{H}_{i, i}=\mu_{i}$. The non-zero off-diagonal entries, $\mathbf{H}_{i, j}=t_{i, j}$, correspond to the hopping elements. We construct the matrix based on the lattice we wish to describe, such that if two sites are neighbours then they have a non-zero hopping between them and zero otherwise.

For example, we can write the Hamiltonian of equation (2.2) as a countably infinite matrix

$$
\mathbf{H}=\left(\begin{array}{lllll}
\ddots & & & & \varnothing  \tag{2.8}\\
& \mu & t & & \\
& t & \mu & t & \\
& & t & \mu & \\
\varnothing & & & & \ddots
\end{array}\right)
$$

### 2.3 Origin of the Tight-binding Model

In the previous section we introduced the tight-binding model, but in order to present a connection to physical systems, we show under what conditions we may derive a tight-binding model from continuum models.
We present two ways to make this derivation, but both have a similar starting point: The wave-function, $\Psi(\vec{r})$, that is a solution of a single particle Schrödinger equation,

$$
\begin{equation*}
\left[\frac{(\mathrm{i} \hbar \vec{\nabla}+e \vec{A})^{2}}{2 m}+U(\vec{r})\right] \Psi(\vec{r})=E \Psi(\vec{r}) \tag{2.9}
\end{equation*}
$$

In this equation the effects of the lattice and disorder are described by the potential $U(\mathbf{r})$. A magnetic field is introduced trough the magnetic vector potential, $\vec{A}$.

To present a more clear derivation, we simplify equation (2.9) by considering a model without magnetic field, $\vec{A}=0$. We reintroduce the magnetic field at the end of this section with Peierls substitution.
The second simplification is to reduce the dimensions to one. The derivation presented in the following sections lends itself to generalisation to multiple dimensions. Thus after these simplifications the starting point are the wave-functions, $\Psi(x)$, that are solutions of the one-dimensional Schrödinger equation,

$$
\begin{equation*}
\left[\frac{-\hbar^{2} \partial_{x}^{2}}{2 m}+U(x)\right] \Psi(x)=E \Psi(x) \tag{2.10}
\end{equation*}
$$

### 2.3.1 Direct Discretization

The most direct way to discretize a wave-function is by choosing a mesh of spacing $a$ and sampling the wave-function at these values

$$
\begin{equation*}
\Psi(x) \rightarrow \Psi(a n)=\Psi_{n} \tag{2.11}
\end{equation*}
$$

where $n$ is a integer. Now we also discretize the Schrödinger equation with the same mesh. The discretization of the kinetic term may be done with finite differences

$$
\begin{equation*}
\frac{-\hbar^{2}}{2 m} \partial_{x}^{2} \Psi(x) \rightarrow \frac{-\hbar^{2}}{2 m a^{2}}\left(2 \Psi_{n}-\Psi_{n-1}-\Psi_{n+1}\right) \tag{2.12}
\end{equation*}
$$

The potential energy term becomes $U(x) \rightarrow U_{n}=U(n a)$. Thus the discretized of equation (2.10) is:

$$
\begin{equation*}
\left(U_{n}+\frac{\hbar^{2}}{m a^{2}}\right) \Psi_{n}-\frac{\hbar^{2}}{2 m a^{2}} \Psi_{n-1}-\frac{\hbar^{2}}{2 m a^{2}} \Psi_{n+1}=E \Psi_{n} \tag{2.13}
\end{equation*}
$$

The underlying assumption in finite differences is that $\Psi(x)$ is smooth on the length scale $a$. This equation is similar in form to equation (2.3), where we described the solutions of an infinite wire in a tight-binding model.
This equation allows us to relate $t$ and $\mu$ to $\hbar, a$ and $m$ by the following relations

$$
\begin{align*}
t & =-\frac{\hbar^{2}}{2 m a^{2}}  \tag{2.14}\\
\mu_{n} & =U_{n}+\frac{\hbar^{2}}{m a^{2}} \tag{2.15}
\end{align*}
$$

In this procedure we introduce discretization error with respect to the original model. One would hope that if $a$ is chosen small enough these errors are negligible, but this is never fully the case as a real space discretization of $a$ is equivalent to introducing a cut-of of $1 / a$ in momentum space. The solutions of the single-particle Schrödinger equation, without potential, are plane waves $\Psi(x) \sim e^{i k x}$, with arbitrarily high
momentum. Thus the discrete model is only identifiable with the continuum model in the low momentum range.

We want to express the range where this connection holds in terms of energy. This will be latter used in establishing a connection for small energies in numerical results. By using equations (2.14) and (2.15) we write the energies of the solutions in the tight-binding and free electron models in terms of $\mu$ and $t$ :

$$
\begin{align*}
E_{\text {Tight binding }} & =\mu+2 t(1-\cos (k a)) \\
& \approx \mu+t(k a)^{2}+O\left((a k)^{4}\right)  \tag{2.16}\\
E_{\text {Free electron }} & =\mu+t(a k)^{2} \tag{2.17}
\end{align*}
$$

where we assumed that $\mu_{n}=\mu$. Concludingly, we may interpret the results of the tight-binding model with the free electron model, if $E-\mu$ is small in units of $t$.

### 2.3.2 Localized Wave-Functions

In the previous section we derived a method for discretizing a nearly free-electron theory, but this procedure relies on the lattice pacing $a$ being negligibly small. This is problematic for the description of the Sierpinski carpet. As when we implement a Sierpinski carpet in the tight-binding model, we remove individual lattice points. When implementing such a lattice, we can not expect the wave-functions to be smooth on the length scale $a$. Thus for the Sierpinski carpet, the free electron discretization can not give physical interpretation, in any regime, to the tight-binding model.

A model that does give physical interpretation for any lattice we use, is based on the wave-functions being heavily localized near the lattice points due to the lattice potential. This is the situation that was drawn in figure 2.4. We connect this model to the tight-binding model by identifying a state $\hat{c}_{i}^{\dagger}|0\rangle$ with a localized wave function $\phi_{i}(\vec{r})$.

In order to more formally derive this identification we need Wannier functions, as those provide the basis of localized wave functions. The Wannier functions are defined in terms of Bloch functions, so we start by a quick recap of the Bloch theorem. The Bloch theorem was first proven by Bloch in 1929 [14]. The theorem states that: If the system we describe has translational symmetry, $\hat{H}(x)=\hat{H}(x+a)$, then we may decompose the solutions of the Schrödinger equation, $\hat{H}(x) \Psi(x)=E \Psi(x)$, into a plane wave and a translationally invariant function,

$$
\begin{equation*}
\Psi_{k}(x)=e^{i k x} u_{k}(x) \tag{2.18}
\end{equation*}
$$

where $u_{k}(x)$ has translational symmetry, $u_{k}(x)=u_{k}(x+a)$.

## Wannier-Functions

The Bloch wave-functions are de-localized solutions with well-defined momentum, but for deriving the equivalence with tight-binding we wish to obtain a description in terms of localized functions. This is done by Fourier-transform the Bloch wave-function to obtain the Wannier-functions,

$$
\begin{equation*}
\phi_{j}(x)=\frac{1}{\sqrt{N}} \sum_{k} e^{-i k j a} \Psi_{k}(x) \tag{2.19}
\end{equation*}
$$

The Wannier functions are orthonormal, which may be proven by an argument following [15]:

$$
\begin{aligned}
\int \phi_{j}^{*}(x) \phi_{j^{\prime}}(x) d x & =\frac{1}{N} \sum_{k, k^{\prime}} \int e^{i k j a} \psi_{k}^{*}(x) e^{-i k^{\prime} j^{\prime} a} \psi_{k^{\prime}}(x) d x \\
& =\frac{1}{N} \sum_{k, k^{\prime}} e^{i a\left(k j-k^{\prime} j^{\prime}\right)} \delta_{k, k^{\prime}} \\
& =\frac{1}{N} \sum_{k} e^{i k a\left(j^{\prime}-j\right)} \\
& =\delta_{j, j^{\prime}}
\end{aligned}
$$

Another useful property of the Wannier functions is that:

$$
\begin{equation*}
\phi_{j}(x)=\phi_{j+1}(x+a) \tag{2.20}
\end{equation*}
$$

This may be proven by combining equations (2.18) and (2.19). The most crucial property we want the Wannier-functions to have is localization, but this is not inherent to the Wannier function definition. This is because Bloch waves are defined up to a phase factor, while the phase factor is not significant in the Bloch-waves, it does influence the localization of the Wannier function. One could for example de-localize a localized Wannier function, by rotating the phase factor of only a single Bloch-function. Nonetheless, we will assume that we have localized Wannier-functions, as these exists and there are methods to maximize the localization of the Wannier functions [16].

## Tight-binding Equivalence

By inverting equation (2.19) we know that Bloch-wave solution may be written as a superposition of Wannierfunctions,

$$
\begin{equation*}
\Psi_{k}(x)=\sum_{j} b_{j} \phi_{j}(x) \tag{2.21}
\end{equation*}
$$

Using the starting point that the Bloch-wave solutions are eigenfunctions of the Hamiltonian,

$$
\begin{equation*}
E \Psi_{k}(x)=H(x) \psi_{k}(x) \tag{2.22}
\end{equation*}
$$

we multiply this equation with a Wannier function, $\phi_{j}^{\dagger}(x)$, and integrate over all space,

$$
\begin{equation*}
\int E \phi_{j}^{\dagger}(x) \Psi(x) d x=\int \phi_{j}^{\dagger}(x) H(x) \Psi(x) d x \tag{2.23}
\end{equation*}
$$

We then insert equation (2.21) and use the orthonormality of Wannier functions to obtain

$$
\begin{aligned}
E b_{j} & =\sum_{j^{\prime}} \int \phi_{j}^{\dagger}(x) H(x) \phi_{j^{\prime}}(x) b_{j^{\prime}} \\
& =\sum_{j^{\prime}} H_{j, j^{\prime}} b_{j^{\prime}}
\end{aligned}
$$

where $H_{j, j^{\prime}}=\int \phi_{j}^{\dagger}(x) H(x) \phi_{j^{\prime}}(x)$. As this is true for arbitrary $j$, we may view this as a matrix equation:

$$
\begin{equation*}
E \vec{a}=\mathbf{H} \vec{b} \tag{2.24}
\end{equation*}
$$

where $\vec{b}=\left(\ldots, b_{j-1}, b_{j}, b_{j+1}, \ldots\right)^{T}$.

We can now identify the matrix $\mathbf{H}$ we derived from the Wannier-functions as in equation (2.24) with the matrix we used to define the general tight-binding models in equation (2.7). In terms of the individual elements this identification means:

$$
\begin{align*}
& \mu_{i}=H_{j, j}  \tag{2.25}\\
&=\int\left|\phi_{j}(x)\right|^{2} H(x) d x  \tag{2.26}\\
& t_{i, j}=H_{i, j}
\end{align*}=\int \phi_{i}^{\dagger}(x) H(x) \phi_{j}(x) d x
$$

The tight-binding model we use only contains nearest neighbour interaction. The nearest neighbours are defined by $H_{i, j} \neq 0$. So if two sites $i$ and $j$ are not neighbours $\int \phi_{i}^{\dagger}(x) H(x) \phi_{j}(x) d x$ should be zero. This is actually not true, but if the Wannier functions are sufficiently localized $\int \phi_{i}^{\dagger}(x) H(x) \phi_{j}(x) d x$ is small enough to justify neglection when the sites are not nearest neighbours.

In order to make the previous argument more tangible, we show how this plays out for the simple wire model as defined in equation (2.2). The hopping from a lattice point $j$ to the lattice point $j+n$ is:

$$
\begin{aligned}
H_{j, j+n} & =\int \phi_{j}^{\dagger}(x) H(x) \phi_{j+n}(x) d x \\
& =\int \phi_{j}^{\dagger}(x) H(x) \phi_{j}(x-n a) d x
\end{aligned}
$$

We assume the Wannier-functions are exponentially localized, meaning: $\phi_{j}(x)<C e^{-|x-j a| / \xi}$, where $\xi$ is some decay length and $C$ some constant. Then $H_{j, j+n} \sim e^{-|n| a / \xi}$. The largest of these hopping terms are to the neighbours, which we identify with the generic hopping parameter $H_{j, j+1}=t$. If we compare $t$ to the other hopping terms, we find that these are at least smaller by a factor $e^{-a / \xi}$, so if $\xi$ is small enough, then there are good grounds for neglecting the terms with $|n| \geq 2$.

## Peierls Substitution

The magnetic field was neglected up till now, but we may reintroduce it through Peierls substitution. The following arguments are inspired by the following reference [17].

We assume that we have a set of Wannier-functions, $\phi_{j}(x)$, that derive from Bloch-functions, $\Psi_{k}(x)$, that are solutions of the Schrödinger equation,

$$
\begin{equation*}
\hat{H}(x) \Psi_{k}(x)=\left[\frac{-\hbar^{2} \partial_{x}^{2}}{2 m}+U(x)\right] \Psi_{k}(x)=E_{k} \Psi_{k}(x) \tag{2.27}
\end{equation*}
$$

Adding a magnetic field changes the Hamiltonian to a new Hamiltonian, $\hat{H}^{A}(x)$,

$$
\begin{equation*}
\hat{H}^{A}(x)=\frac{\left(\mathrm{i} \hbar \partial_{x}+e A_{x}\right)^{2}}{2 m}+U(x) \tag{2.28}
\end{equation*}
$$

We introduce a new set of Wannier-functions, $\phi_{j}^{A}(x)$, that are related to the old Wannier-functions by a phase,

$$
\begin{equation*}
\phi_{j}^{A}(x)=e^{i \frac{e}{\hbar} \int_{j a}^{x} A_{x} d x} \phi_{j}(x) \tag{2.29}
\end{equation*}
$$

These phases are chosen such that the momentum operator, $\mathrm{i} \hbar \partial_{x}$, acting on the phase gives $-e A_{x}$. This allows us to write the Hamiltonian with magnetic field, $\hat{H}^{A}$, acting on the new Wannier-function, $\phi_{j}^{A}$, as the
old Hamiltonian acting on the old-Wannier function

$$
\begin{align*}
\hat{H}^{A}(x) \phi_{j}^{A}(x) & =\left[\frac{\left(\mathrm{i} \hbar \partial_{x}+e A_{x}\right)^{2}}{2 m}+U(x)\right] e^{i \frac{e}{\hbar} \int_{j a}^{x} A_{x} d x} \phi_{j}(x) \\
& =e^{i \frac{e}{\hbar} \int_{j a}^{x} A_{x} d x}\left[\frac{\left(\mathrm{i} \hbar \partial_{x}+e A_{x}-e A_{x}\right)^{2}}{2 m}+U(x)\right] \phi_{j}(x)  \tag{2.30}\\
& =e^{i \frac{e}{\hbar} \int_{j a}^{x} A_{x} d x} \hat{H}(x) \phi_{j}(x)
\end{align*}
$$

The effect of changing the Wannier-function on the hopping is:

$$
\begin{align*}
t^{A}=H_{j, j+1}^{A} & =\int \phi_{j}^{A \dagger}(x) \hat{H}^{A}(x) \phi_{j+1}^{A}(x) d x \\
& =\int e^{i \frac{e}{\hbar}\left(\int_{(j+1) a}^{x} A_{x} d x-\int_{j a}^{x} A_{x} d x\right)} \phi_{j}^{\dagger}(x) H(x) \phi_{j+1}(x) d x  \tag{2.31}\\
& =e^{i \frac{e}{\hbar} \int_{(j+1) a}^{j a} A_{x} d x} t
\end{align*}
$$

So the effect of the magnetic field in a tight-binding model is that it changes the hopping by a phase factor that depends on the gauge field.

### 2.4 Integer Quantum Hall Effect



Figure 2.5: Sketch of the classical Hall effect.
In this section we derive and discuss the integer quantum Hall effect, but first we give a brief introduction to the classical Hall effect. The classical Hall effect happens when a sheet of metal is put in a magnetic field and one drives a current through this sheet of metal. The electrons travelling in the sheet of metal are deflected to the edges due to Lorentz force. As electrons build up at an edge, they generate a electric field that counteracts the Lorentz force. When the system is in equilibrium the current can travel trough the sheet, but if one where to measure the voltage between the edges of the sheet, one finds that there is a voltage drop, this voltage is called the Hall voltage, $V_{H}$. We illustrate the situation in figure 2.5.

From the classical Hall effect we obtain the prediction that $\rho_{x, x}$ is constant and $\rho_{x, y}$ increases linearly with the magnetic field [18]. Yet in experiments performed by von Klitzing in 1980 it was found that when the magnetic field is sufficiently large, $\rho_{x, y}$ is made up of plateaus and $\rho_{x, x}$ is nearly zero except when the plateaus change, this is called the integer Hall effect [19].

The integer Hall effect may be explained by using the non-interacting Schrödinger equation. We consider a free particle Hamiltonian with a magnetic field

$$
\begin{equation*}
\hat{H}=\frac{1}{2 m}(\vec{p}+e \vec{A})^{2} \tag{2.32}
\end{equation*}
$$



Figure 2.6: Left: Prediction of the classical Hall effect. Right: Example of the integer Hall effect [18]

We choose the Landau gauge to introduce the magnetic field

$$
\begin{equation*}
\vec{A}=(0, x B, 0) . \tag{2.33}
\end{equation*}
$$

In Landau gauge, the Hamiltonian of equation 2.32 is

$$
\begin{equation*}
\hat{H}=\frac{1}{2 m}\left(\hat{p}_{x}^{2}+\left(\hat{p}_{y}+e B \hat{x}\right)^{2}\right) \tag{2.34}
\end{equation*}
$$

As this Hamiltonian is translationally invariant in the $y$ direction, we have that the commutator for the Hamiltonian and the translation operator in the $y$ direction is zero, $\left[\hat{H}, \hat{T}_{y}(a)\right]=0$. This means there is a basis of energy eigenstates that are also translationally invariant, up to a phase factor, in the $y$ direction

$$
\begin{equation*}
\psi_{k}(x, y)=e^{-i k y} f_{k}(x) \tag{2.35}
\end{equation*}
$$

Using these wave-functions to find the energies gives

$$
\begin{equation*}
\hat{H} \psi_{k}(x, y)=\frac{1}{2 m}\left(\hat{p}_{x}^{2}+(\hbar k+e B \hat{x})^{2}\right) \psi_{k}(x, y) \tag{2.36}
\end{equation*}
$$

This equation may be rewritten into a quantum harmonic oscillator with a shifted minimum,

$$
\begin{equation*}
\hat{H} \psi_{k}(x, y)=\left(\frac{1}{2 m} \hat{p}_{x}^{2}+\frac{m \omega_{B}^{2}}{2}\left(\hat{x}-k l_{B}^{2}\right)^{2}\right) \psi_{k}(x, y) \tag{2.37}
\end{equation*}
$$

where $\omega_{B}=e B / m$ and $\left.l_{B}^{2}=\hbar /(e B)\right)$. This is an equation for a quantum harmonic oscillator with the minimum of the potential shifted to $k l_{B}^{2}$, but this shift has no influence on the energy. The quantum harmonic oscillator energies are

$$
\begin{equation*}
E_{n}=\hbar \omega_{B}\left(n+\frac{1}{2}\right) \tag{2.38}
\end{equation*}
$$

Because the energy has no dependence on $k$, there is a degeneracy at every energy level $E_{n}$ that looks like

where $\mu$ is the chemical potential. The empty dots represent the states being empty and the filled dots represent filled states. The energy plateaus are called landau levels and they allow us to explain the behaviour of $\rho_{x, x}$. In order a system to be conducting, there must be states close to the chemical potential, where the definition of close is related to the temperature. This is only true if the chemical potential is approximately equal to a Landau level

$$
\begin{equation*}
\mu \approx E_{n}=\hbar \omega_{B}\left(n+\frac{1}{2}\right) \tag{2.39}
\end{equation*}
$$

This is only true for specific values of the magnetic field, thus explaining the conductivity peaks and insulating behaviour otherwise.

To explain the effect on the Hall resistivity, $\rho_{x, y}$, we need to introduce two edges. This allows us to define a voltage gap across the edges. We can create edges in our system by introducing a potential field $V(x)$ that is flat in the bulk of the material and rises at the edges


This potential smoothly terminates the system by increasing the potential until it is above the chemical potential $\mu$ and no filled states exist in that region, thus introducing a boundary for the electrons.

To solve the system with a potential, we use that the solutions of the system without potential are strongly localized. This follows from the solutions of the quantum harmonic oscillator. These allow us to solve the profile in the $x$ direction for $\Psi_{n, k}(x)$

$$
\begin{equation*}
\Psi_{n, k}(x) \sim e^{i k y} e^{\frac{\left(x-k l_{B}^{2}\right)^{2}}{2 l_{B}^{2}}} H_{n}\left(l_{B}^{-2}\left(x-k l_{B}^{2}\right)\right) \tag{2.40}
\end{equation*}
$$

where $H_{n}(x)$ is the $n$th hermite polynomial. These solutions are exponentially localized in the $x$ direction, centred at $k l_{B}^{2}$. If the potential $V(x)$ changes slowly in comparison to the length-scale of the solutions, $l_{B}$, we may treat the effects of the potential as a constant energy shift for each solution. Thus, depending on the $k$ of the solution, the potential is $V(x) \approx V\left(k l_{B}^{2}\right)$. Such that the energy of the Landau levels becomes $k$ dependant

$$
\begin{equation*}
E_{n, k}=\hbar \omega_{B}\left(n+\frac{1}{2}\right)+V\left(k l_{B}^{2}\right) \tag{2.41}
\end{equation*}
$$

We may visualise the influence of the potential on the states of a single Landau level in the picture below


We can introduce a Hall voltage into our system by creating a potential difference between the two edges such that $e V_{H}=\mu_{1}-\mu_{2}$. This changes the occupation of the states near the edges


Due to this difference in occupation there is now a current in the $y$ direction. We derive this by using the group velocity, where we take the derivative of equation (2.41) to $k$

$$
\begin{equation*}
v_{y}=\frac{1}{\hbar} \frac{\partial E_{n, k}}{\partial k}=\frac{l_{B}^{2}}{\hbar} \frac{\partial V}{\partial x} . \tag{2.42}
\end{equation*}
$$

For the second line we used the localization of the states to identify $x$ to $k$ by $x=k l_{B}^{2}$. We find the total current by integrating over all states $k$ that are filled

$$
\begin{equation*}
I_{y}=-e \int_{\text {filled states }} \frac{d k}{2 \pi} v_{y}=\frac{e}{2 \pi l_{B}^{2}} \int_{\text {filled states }} d x \frac{l_{B}^{2}}{\hbar} \frac{\partial V}{\partial x}=\frac{e}{2 \pi \hbar}\left(\mu_{1}-\mu_{2}\right) \tag{2.43}
\end{equation*}
$$

So we obtain an expression for the Hall conductivity for a single Landau level

$$
\begin{equation*}
\sigma_{x y}=\frac{I_{y}}{\Delta V_{x}}=\frac{e^{2}}{2 \pi \hbar} \tag{2.44}
\end{equation*}
$$

For multiple Landau levels the same picture holds, but with each Landau level shifted by $\hbar \omega_{B}$, as we display below


For each filled Landau level one may repeat the same calculation and each level contributes the same value to the conductivity. So for the full system the Hall conductivity is

$$
\begin{equation*}
\sigma_{x y}=\frac{e^{2}}{2 \pi \hbar} n_{\text {filled }} \tag{2.45}
\end{equation*}
$$

where $n_{\text {filled }}$ is the amount of filled Landau levels. So now we can explain the behaviour of the Hall resistivity, $\sigma_{x y}$, as seen in figure 2.6. The spikes in $\rho_{x x}$ happen because the chemical potential is approximately at a landau level, so there is conduction in the bulk of the material. The Hall resistivity is completely determined by the amount of filled landau levels. As the spikes in $\rho_{x x}$ correspond to a change in the amount of filled Landau levels this is the only place where the Hall resistivity changes.

If the potential $V(x)$ is shaped such that $V(x)=V_{0}$ inside the bulk of the material and only becomes $x$ dependant near the edge, then the current $I_{y}$ is fully generated by states on the edge. Even more important: on the left edge the derivative of the potential is negative, $\frac{\partial V}{\partial x}<0$, while on the right edge it is positive ,$\frac{\partial V}{\partial x}>0$. As the group velocity is proportional to this derivative of the potential, the velocity of the states on the left edge is opposite of the states on the right edge. Thus we have chiral edge modes, where the modes on the edge only travel in a single direction. If the system also has edges in the $y$ directions, we also obtain the same effect on these edges. This means that if the bulk of the system is isolating, all transport takes place along the edges. These edges only support transport in one direction, that depends on the orientation of the magnetic field:


An important property of the integer Hall effect is that it does not depend on the specifics of the edge and is stable to impurities. This can be explained in multiple ways. Because at the edges the states move in a single direction, when an electron encounters an impurity along the edge and scatters, it can only scatter into other modes that also move in the same direction. Thus the chiral edge modes provide perfect channels
for transport around the edge.
The second explanation lies in the way we calculated the Hall conductance. Nowhere in the calculation did we have to specify the exact profile of the potential $V(x)$. The only properties used are: $V(x)$ rises at the edges and $V(x)$ is smooth on the length scale $l_{B}$. Thus any impurities, which we would describe by a profile in $V(x)$, do not influence the conductance, as long as the description of Landau levels remains unaffected.

For the last explantation we note that this system is a topological insulator. Topological insulators are systems where the bulk of the system is insulating. For this inner region one may calculate a topological quantity over the filled bands, which is integer valued. For the integer quantum Hall effect this topological quantity is the Chern number and each filled Landau level contributes exactly one to the Chern number. At the edges of topological insulators, where the topological quantity changes value, this gives rise to special edge modes. The presence and properties of these edge modes is determined by the topological quantity and not by any specifics of the edge. As the topological quantity is determined by the bands in the bulk of the system and it only changes when the system becomes conducting, the properties of the edge modes are very stable [18, 20, 3].

## Chapter 3

## Theoretical Framework

### 3.1 Introduction

The main goal of this thesis is to find the conductance through a device that is coupled to two semiinfinite leads, as shown in figure 3.1. This chapter is devoted to explaining the method used to calculate the conductance. We begin this chapter with the introduction of the Landauer-Büttiker formalism. The Landauer-Büttiker formalism reduces the problem of calculating conductance to finding the transmission function, $T(E)$. This transmission function depends on two types of Green's functions: The Green's functions from the edge of the left lead of the device to the right lead. The second type of Green's function are the surface Green's function for the uncoupled semi-infinite leads. To solve both of these Green's functions we introduce the recursive Green's function formalism, which is used to solve the Green's functions of the semi-infinite leads analytically and it provides a numerical scheme to compute the other Green's function.

### 3.2 Landauer-Büttiker formalism



Figure 3.1: Schematic diagram of the set-up of the two-terminal wire we use the Landauer-Büttiker formalism to compute linear response conductivity.

In order to calculate the current, we use the Landauer-Büttiker formalism [21, 22]. This provides an equation for the current

$$
\begin{equation*}
I=\frac{-e}{h} \int T(E)\left[f_{L}(E)-f_{R}(E)\right] d E \tag{3.1}
\end{equation*}
$$

where $e$ is the electric charge, $h$ is Planck's constant, $T(E)$ is the Transmission function from the left lead to the right lead and $f_{L / R}(E)$ are the Fermi-Dirac distributions in the left and right leads,

$$
\begin{equation*}
f_{L / R}(E)=\left[1+e^{\beta_{L / R}\left(E-\mu_{L / R}\right)}\right]^{-1} \tag{3.2}
\end{equation*}
$$

The transmission function, $T(E)$, is related to scattering matrices from the left lead to the right lead of the modes at an energy $E . T(E)$ may be interpreted as a likelihood that a mode at energy $E$ from the left lead can enter a mode at the same energy in the right lead.

Combined with the Fermi-Dirac distributions, $f_{L}(E)$, which contain the information on how many modes are occupied at this energy, we may interpret $T(E) f_{L}(E)$ as the amount of electrons at energy $E$ hopping from the left lead to the right lead. $T(E) f_{R}(E)$ is the amount of electrons hopping in the reverse direction, thus $T(E)\left(f_{L}(E)-f_{R}(E)\right)$ is the nett change of electrons between the leads at a specific energy. Thus integrating it over energy gives the total current.

In the limit of temperature to zero, $\beta_{L}=\beta_{R} \rightarrow \infty$, the Fermi-Dirac functions become step-functions

$$
\lim _{\beta \rightarrow \infty} f_{L / R}(E)= \begin{cases}1, & \text { for } E>\mu_{L / R}  \tag{3.3}\\ 0, & \text { for } E<\mu_{L / R}\end{cases}
$$

This changes equation (3.1) to

$$
\begin{equation*}
I=\frac{-e}{h} \int_{\mu_{L}}^{\mu_{R}} T(E) d E \tag{3.4}
\end{equation*}
$$

When the difference of the chemical potential, $\mu_{L}-\mu_{R}$, is sufficiently small, such that the transmission function $T_{L R}(E)$ is approximately constant over the interval $\mu_{L}$ to $\mu_{R}$, then we recover an equation for linear response

$$
\begin{equation*}
I=\frac{e^{2}}{h} T\left(E_{F}\right)\left(V_{L}-V_{R}\right) \tag{3.5}
\end{equation*}
$$

where $E_{F} \approx \mu_{L} \approx \mu_{R}$ and $V_{L / R}=\mu_{L / R} / e$.
In this linear response regime the transmission function is directly related to the conductance across the device

$$
\begin{equation*}
\sigma_{x x}=\frac{I}{\Delta V}=\frac{e^{2}}{h} T\left(E_{F}\right) \tag{3.6}
\end{equation*}
$$

### 3.2.1 Green's functions

To compute the transmission, $T(E)$, we need Green's functions. This section provides a brief introduction to Green's functions as far as necessary for the computation of the transmission.

For a general system, where we have a Hamiltonian, $\hat{H}$, the Green's function $\hat{G}(E)$ is defined as the inverse operator of the energy, $E$, minus the Hamiltonian

$$
\begin{equation*}
(E \hat{1}-\hat{H}) \hat{G}(E)=\hat{1} \tag{3.7}
\end{equation*}
$$

The physical interpretation of this operator may be shown by solving the equation

$$
\begin{equation*}
(E \hat{1}-\hat{H}) \psi_{n}^{\prime}(x)=f(x) \tag{3.8}
\end{equation*}
$$

If we assume that we already had a solution $\psi_{n}$ of $\hat{H}$, such that $\hat{H} \psi_{n}=E_{n} \psi_{n}$. Then we can define $\psi_{n}^{\prime}(x)=\psi_{n}(x)+\hat{G}(E) f(x)$. Using this to solve equation (3.8), we obtain

$$
\begin{aligned}
f(x) & =(E \hat{1}-\hat{H}) \psi(x) \\
& =\left(E-E_{n}\right) \psi_{n}(x)+\hat{1} f(x)
\end{aligned}
$$

This is true if $E=E_{n}$. So $\psi(x)=\psi_{n}(x)+\hat{G}\left(E_{n}\right) f(x)$ is a solution of equation (3.8).
The interpretation of $f(x)$ in equation (3.8) is that it acts like a sink or source depending on the sign. So $\hat{G}(E)$ describes the response of solutions of energy $E$ to a sink or source.

This way of looking at Green's functions works for many classical system, such as electrostatics [23], but it fails if we wish to describe a countable quantum-mechanical system. When we have a set of solutions $\hat{H}\left|\psi_{n}\right\rangle=E_{n}\left|\psi_{n}\right\rangle$, then the Green's function is

$$
\begin{equation*}
\hat{G}(E)=\sum_{n} \frac{\left|\psi_{n}\right\rangle\left\langle\psi_{n}\right|}{E-E_{n}} \tag{3.9}
\end{equation*}
$$

This undefined for $E=E_{n}$. The solution to the undefined Green's function, is to introduce the retarded, $\hat{G}^{+}(E)$, and advanced, $\hat{G}^{-}(E)$, Green's functions [22]:

$$
\begin{equation*}
\hat{G}^{ \pm}(E)=\lim _{\eta \rightarrow 0^{+}} \frac{1}{(E \pm i \eta) \hat{1}-\hat{H}} \tag{3.10}
\end{equation*}
$$

The retarded and advanced Green's functions are linked to causal and anti-causal two point functions by Fourier-transformation in the energy-time domain [24].

In this thesis we work in a position basis for the Green's function, as such we can group the elements into a matrix, $\mathbf{G}(E)$, where the individual elements of the matrix are

$$
\begin{equation*}
\mathbf{G}(E)_{i j}=\langle i| \hat{G}(E)|j\rangle . \tag{3.11}
\end{equation*}
$$

Because the Hamiltonian in our models can always be expressed as a matrix, see equation (2.7), the Green's function is the matrix inverse of $E \mathbf{1}-\mathbf{H}$ and likewise for the retarded and advanced Green's functions

$$
\begin{equation*}
\left.\mathbf{G}^{ \pm}(E)=\lim _{\eta \rightarrow 0^{+}}((E \pm i \eta) \mathbf{1})-\mathbf{H}\right)^{-1} \tag{3.12}
\end{equation*}
$$

A property of the retarded and advanced Green's functions we will use in te next section is that $\hat{G}^{+}=\left(\hat{G}^{-}\right)^{\dagger}$ as $\hat{H}=\hat{H}^{\dagger}$, so only the sign of $i \eta$ flips. So the Green's function matrices are also related to each other by hermitian conjugation

$$
\begin{equation*}
\mathbf{G}_{i, j}^{-}=\left(\mathbf{G}_{j, i}^{+}\right)^{\dagger} \tag{3.13}
\end{equation*}
$$

### 3.2.2 Transmission function

In the previous section we described how the conductance may be related to the transmission function, $T(E)$. In this section we give an overview of the method used to calculate the transmission function and reduce the problem into that of finding the green's functions.

The formula for the transmission function in a tight binding model is given by [25]:

$$
\begin{equation*}
T(E)=\operatorname{Tr}\left[\boldsymbol{\Gamma}_{L}(E) \mathbf{G}_{L R}^{+}(E) \boldsymbol{\Gamma}_{R}(E) \mathbf{G}_{R L}^{-}(E)\right] \tag{3.14}
\end{equation*}
$$



Figure 3.2: Schematic diagram showing the elements in equation (3.14). Both of the arrows in the left lead belong to $\Gamma_{L}(E)$. Likewise for the right lead. The solid black lines represents the edges of the device.

All objects in this equation are matrices, where the indices refer to sites on either the left or the right edge of the device. $\mathbf{G}_{L R}^{+}(E)$ is a matrix containing the retarded green's functions from the left edge to the right edge. $\mathbf{G}_{R L}^{-}(E)$ contains the advanced greens function from the right edge to the left edge.

The green's functions may be thought of as propagators from one edge of the device to the other edge. This identification is represented in figure 3.2 as the arrows between the edges.

By using equation (3.13), we may relate $\mathbf{G}_{R L}^{-}(E)$ to $\mathbf{G}_{L R}^{+}(E)$ by hermitian conjugation:

$$
\begin{equation*}
\mathbf{G}_{R L}^{-}(E)=\left(\mathbf{G}_{L R}^{+}(E)\right)^{\dagger} \tag{3.15}
\end{equation*}
$$

Thus it is sufficient to find $\mathbf{G}_{L R}^{+}(E)$.

The functions $\boldsymbol{\Gamma}_{L}(E)$ and $\boldsymbol{\Gamma}_{R}(E)$ are called the broadening functions and they are matrices where both indices refer to sites on the same edge of the device. The broadening functions contain information about the modes in the semi-infinite leads, such as the transverse profile that is presented to the edge of the device and the density of a mode. We represent them in figure 3.2 by incoming and outgoing arrows inside the leads, as the broadening functions describe the transport in the leads.

We may also express the broadening functions in terms of green's functions by first writing it in terms of the self-energy, $\boldsymbol{\Sigma}_{L / R}$ :

$$
\begin{equation*}
\boldsymbol{\Gamma}_{L / R}(E)=i\left(\boldsymbol{\Sigma}_{L / R}-\boldsymbol{\Sigma}_{L / R}^{\dagger}\right) \tag{3.16}
\end{equation*}
$$

The self-energies, $\boldsymbol{\Sigma}_{L / R}$, in turn depends on the surface green's functions, $\mathbf{g}_{L / R}^{+}(E)$,

$$
\begin{equation*}
\boldsymbol{\Sigma}_{L / R}=\mathbf{V}_{L / R} \mathbf{g}_{L / R}^{+}(E) \mathbf{V}_{L / R}^{\dagger} \tag{3.17}
\end{equation*}
$$

Here $\mathbf{V}_{L / R}$ is a matrix containing the hopping terms between the edge of the device and the edge of the lead. $\mathbf{g}_{L / R}^{+}(E)$ contains the retarded green's functions from the edge of the lead to the same edge of the lead, but without the device connected to the lead.

### 3.3 Recursive Green's Function Method

The recursive Green's function method is a method for "glueing" lattices in a tight binding formalism. In this section we derive the recursive equations, which we will use to perform the calculation of the Green's function to find the transmission. The derivation of these equations starts with the introduction of the

Dyson's equation, that describes the response of the Green's function when the Hamiltonian is changed.

### 3.3.1 Dyson's Equation

We begin the explanation of Dyson's equation, by first introducing two tight binding models that may be described by matrices $\mathbf{H}_{\text {old }}$ and $\mathbf{H}_{\text {new }}$. These two models are related to each other by:

$$
\begin{equation*}
\mathbf{H}_{\text {new }}=\mathbf{H}_{\mathrm{old}}+\mathbf{V} \tag{3.18}
\end{equation*}
$$

This formalism may be used for any system that can be represented by the matrices $\mathbf{H}_{\text {old }}$ and $\mathbf{H}_{\text {new }}$, but our focus is on systems where the old Hamiltonian, $\mathbf{H}_{\text {old }}$, contains two unconnected subsystems

$$
\mathbf{H}_{\mathrm{old}}=\left(\begin{array}{cc}
\mathbf{H}_{1} & 0  \tag{3.19}\\
0 & \mathbf{H}_{2}
\end{array}\right)
$$

and the elements that are introduced, $\mathbf{V}$, containing only terms connecting the two systems

$$
\mathbf{V}=\left(\begin{array}{cc}
0 & \mathbf{V}_{12}  \tag{3.20}\\
\mathbf{V}_{21} & 0
\end{array}\right)
$$

An example of such a system is shown in figure 3.3.


Figure 3.3: Schematic diagram of both the Dyson equation as we explain in this thesis and the main idea of the recursive Green's function method.

We define the Green's functions $g$ and $G$ for the systems $\mathbf{H}_{\text {old }}$ and $\mathbf{H}_{\text {new }}$ by:

$$
\begin{align*}
\mathbf{g} & =\left(E \mathbf{1}-\mathbf{H}_{\text {old }}\right)^{-1}  \tag{3.21}\\
\mathbf{G} & =\left(E \mathbf{1}-\mathbf{H}_{\text {new }}\right)^{-1} \tag{3.22}
\end{align*}
$$

By using these equations and equation (3.18), we may derive Dyson's equation [24]

$$
\begin{equation*}
\mathbf{G}=\mathbf{g}+\mathbf{g V G} \tag{3.23}
\end{equation*}
$$

Dyson's equation is not closed, but it can be used to generate a set of equations that are closed. To write these equations we must first introduce a new way of grouping the Green's functions.

This grouping is done by dividing the system into slices labelled by an integer, $i \in\{1,2, \ldots, N-1, N\}$. Here the slice 1 is the slice connected to the left lead and slice $N$ the slice connected to the right lead, which is


Figure 3.4: Schematic diagram of how the slices are defined.
shown in figure 3.4. Then we extend this to the Green's functions so that $\left(\mathbf{G}_{n m}(E)\right)_{i j}$ refers to the Green's function from site $i$ in slice $n$ going to site $j$ in slice $m$. In this way of writing Green's functions we identify the Green's function connecting the left lead tot the right lead, as the Green's function from slice 1 to slice $N, \mathbf{G}_{L R}(E)=\mathbf{G}_{1 N}(E)$.

We also introduce projection operators $\mathcal{P}_{n} . \mathcal{P}_{n}$ projects only the site belonging to slice $n$. So we identify $\mathbf{G}_{n m}(E)=\mathcal{P}_{n} G(E) \mathcal{P}_{m}^{\dagger}$. Also note that $1=\sum_{n} \mathcal{P}_{n} \mathcal{P}_{n}^{\dagger}$.

### 3.3.2 Recursive Green's Function Equations

The recursive Green's function method is about glueing lattices together as we have shown with Dyson's equation in figure 3.4, while Dyson's equations are not closed, the recursive equations are. Furthermore in the recursive equations we always connect slices.

Each recursive step starts with a system composed of $n$ slices that are connected and a slice $n+1$ that is unconnected from the rest. For this system the matrices $\mathbf{g}_{n, n}, \mathbf{g}_{1, n}$ and $\mathbf{g}_{n+1, n+1}^{-1}$ are known. We have matrices containing the hopping to be introduced between slice $n$ and slice $n+1$, in the form of the matrices $\mathbf{V}_{n+1, n}$ and $\mathbf{V}_{n, n+1}=\mathbf{V}_{n+1, n}^{\dagger}$.

The recursive equations (3.25) and (3.24) allow for the computation of $\mathbf{G}_{1, n+1}$ and $\mathbf{G}_{n+1, n+1}$. $\mathbf{G}_{1, n+1}$ and $\mathbf{G}_{n+1, n+1}$ are then used as the initial matrices $\mathbf{g}$ for the next step in the calculation. The procedure is graphically summarized in figure 3.5 .
The recursive Green's function equations are:

$$
\begin{align*}
\mathbf{G}_{1, n+1} & =\mathbf{g}_{1, n} \mathbf{V}_{n, n+1} \mathbf{G}_{n+1, n+1},  \tag{3.24}\\
\mathbf{G}_{n+1, n+1} & =\left(\mathbf{g}_{n+1, n+1}^{-1}-\mathbf{V}_{n+1, n} \mathbf{g}_{n, n} \mathbf{V}_{n, n+1}\right)^{-1} \tag{3.25}
\end{align*}
$$




Figure 3.5: Overview of a recursive step.

## Deriving the Recursive Green's Function Equations

The goal in of the recursive equations is to find an equation for $\mathbf{G}_{1, N}(E)$ of the fully connected system, it is sufficient to obtain a recursive equation for $\mathbf{G}_{1, n+1}(E)$ in terms of $\mathbf{g}_{1, n}(E)$. It turns out that this equation also requires $\mathbf{g}_{n n}(E)$, thus we also require a recursive equation for $\mathbf{G}_{n+1, n+1}(E)$.

We obtain an equation for $\mathbf{G}_{1, n+1}(E)$ by multiplying Dyson's equation with $\mathcal{P}_{1}$ from the left and $\mathcal{P}_{n+1}$ from the right

$$
\begin{aligned}
\mathbf{G}_{1, n+1} & =\mathcal{P}_{1} \mathbf{G} \mathcal{P}_{n+1}^{\dagger} \\
& =\mathcal{P}_{1} \mathbf{g} \mathcal{P}_{n+1}^{\dagger}+\sum_{j, k} \mathcal{P}_{1} \mathbf{g} \mathcal{P}_{j}^{\dagger} \mathcal{P}_{j} \mathbf{V} \mathcal{P}_{k}^{\dagger} \mathcal{P}_{k} \mathbf{G} \mathcal{P}_{n+1}^{\dagger} \\
& =\mathbf{g}_{1, n+1}+\sum_{j, k} \mathbf{g}_{1, j} \mathbf{V}_{j, k} \mathbf{G}_{k, n+1} \\
& =\mathbf{g}_{1, n} \mathbf{V}_{n, n+1} \mathbf{G}_{n+1, n+1}
\end{aligned}
$$

Here $\mathbf{g}_{1, n+1}$ is zero because $\mathbf{g}$ has no connection from slice 1 to slice $n+1$. The sums over $j$ and $k$ could be reduced because only $\mathbf{V}_{n, n+1}$ and $\mathbf{V}_{n+1, n}$ are not zero, but as $\mathbf{g}_{1, n+1}$ is zero, only the term with $\mathbf{V}_{n, n+1}$ remains.

We repeat the previous calculation for $\mathbf{G}_{n+1, n+1}$ and $\mathbf{G}_{n, n+1}$ to obtain the equations:

$$
\begin{align*}
\mathbf{G}_{n+1, n+1} & =\mathbf{g}_{n+1, n+1}+\mathbf{g}_{n+1, n+1} \mathbf{V}_{n, n+1} \mathbf{G}_{n, n+1}  \tag{3.26}\\
\mathbf{G}_{n, n+1} & =\mathbf{g}_{n, n} \mathbf{V}_{n, n+1} \mathbf{G}_{n+1, n+1} \tag{3.27}
\end{align*}
$$

By combining and rewriting the previous two equations, a closed equation for $\mathbf{G}_{n+1, n+1}$ is obtained:

$$
\begin{equation*}
\mathbf{G}_{n+1, n+1}=\left(\mathbf{g}_{n+1, n+1}^{-1}-\mathbf{V}_{n+1, n} \mathbf{g}_{n, n} \mathbf{V}_{n, n+1}\right)^{-1} \tag{3.28}
\end{equation*}
$$

This allows us to solve the equation for $\mathbf{G}_{1, n+1}(E)$.

### 3.4 Surface Green's Functions

### 3.4.1 Symmetry of the Semi-Infinite Wire

With the recursive Green's function equations we can analytically solve the surface Green's functions, but first a small note about translational symmetry in a semi-infinite system must be made. Translational
symmetry as we know it in the infinite system is absent, as any site has a finite distance to the edge and a translation changes this distance. But a translation in a semi-infinite wire is a symmetry if we combine it with the addition or removal of the appropriate number of sites. An example of this is shown in the figure below


We use this symmetry for solving the semi-infinite wire analytically as we show in the next section.

### 3.4.2 Solving the Semi-Infinite Wire

To describe the influence of the semi-infinite wire we only need the surface Green's functions, $\mathbf{G}_{\text {surface }}$. In the slices formalism a semi-infinite wire is a set of connected slices starting at an arbitrary slice number, which we define as $n$, with an infinite number of identical slices into the $-\infty$ direction. So the surface Green's function in the slices formalism is $\mathbf{G}_{\text {surface }}=\mathbf{G}_{n, n}$.

To obtain an equation for $\mathbf{G}_{\text {surface }}$ we use the symmetry of the semi-infinite wire as explained above. This symmetry implies that $\mathbf{g}_{n, n}$ is equal to $\mathbf{G}_{n+1, n+1}$, if we add a slice using the recursive equations.

We obtain an equation for $\mathbf{G}_{\text {surface }}$ by using $\mathbf{G}_{\text {surface }}=\mathbf{G}_{n+1, n+1}=\mathbf{g}_{n, n}$ to write the recursive surface equation (3.25) as

$$
\begin{equation*}
\mathbf{G}_{\text {surface }}=\left(\mathbf{g}_{n+1, n+1}^{-1}-\mathbf{V}_{n+1, n} \mathbf{G}_{\text {surface }} \mathbf{V}_{n, n+1}\right)^{-1} \tag{3.29}
\end{equation*}
$$

This equation is further simplified by using the square lattice structure in the leads. In a square lattice hopping from slice $n$ to slice $n+1$ only takes place between sites of the same index. Furthermore the hopping, $t$, is identical for all slices and sites. So $\mathbf{V}_{n+1, n}=\mathbf{V}_{n, n+1}=t \mathbf{1} . \mathbf{g}_{n+1, n+1}^{-1}$ is the unconnected slice inverse Green's function $\mathbf{g}_{n+1, n+1}^{-1}=E \mathbf{1}-\mathbf{H}_{\text {lead }}$, where $\mathbf{H}_{\text {lead }}$ is the Hamiltonian for an unconnected slice in the lead. Using these statements, equation (3.29) is

$$
\begin{equation*}
\mathbf{G}_{\text {surface }}\left(E \mathbf{1}-\mathbf{H}_{\text {lead }}\right)-t^{2} \mathbf{G}_{\text {surface }} \mathbf{G}_{\text {surface }}=\mathbf{1} \tag{3.30}
\end{equation*}
$$

The solution for a general wire of width $W$ may be obtained by going to a basis in which $\mathbf{H}_{\text {lead }}$ is diagonal:

$$
\begin{equation*}
\mathbf{S}^{\dagger} \mathbf{H}_{\text {lead }} \mathbf{S}=\operatorname{diag}\left(E_{1}, E_{2}, \ldots, E_{W}\right) \tag{3.31}
\end{equation*}
$$

With $\mathbf{S}$ the matrix with rows corresponding to the eigenvectors of $\mathbf{H}_{\text {lead }}$.
We may assume that in this basis the solution, $\mathbf{G}_{\text {surface }}$, is also diagonal:

$$
\begin{equation*}
\mathbf{S}^{\dagger} \mathbf{G}_{\text {surface }} \mathbf{S}=\operatorname{diag}\left(G_{1}, G_{2}, \ldots, G_{W}\right) \tag{3.32}
\end{equation*}
$$

Then by multiplying equation (3.30) with $\mathbf{S}^{\dagger}$ from the left, $\mathbf{S}$ from the right and using $\mathbf{S}^{\dagger} \mathbf{S}=\mathbf{1}$, we obtain $W$ decoupled equations:

$$
\begin{equation*}
\left(E-E_{w}\right) G_{w} \pm t^{2} G_{w}^{2}=1 \tag{3.33}
\end{equation*}
$$

where $w \in\{1, \ldots, W\}$. Thus the solution for $G_{w}$ are

$$
\begin{equation*}
t G_{w}=\left(E-E_{w}\right) / 2 t \pm i \sqrt{1-\left(\left(E-E_{w}\right) / 2 t\right)^{2}} \tag{3.34}
\end{equation*}
$$

We always choose the negative solution, as the density of states in the leads is minus the imaginary part of the Green's function.
So the solution for the surface Green's function is

$$
\begin{equation*}
\mathbf{G}_{\text {surface }}=\mathbf{S} \operatorname{diag}\left(G_{1}, G_{2}, \ldots, G_{W}\right) \mathbf{S}^{\dagger} \tag{3.35}
\end{equation*}
$$

### 3.5 Computing Transmission

In the previous chapter we have established the theoretical framework necessary to compute the transmission or conductance in a tight binding model. This was done in a top down manner, to provide a narrative to follow. In this section we bring all component together to compute the transmission.

The starting point of any calculation is to specify a width $W$ of the model we describe, a length $N$ of the device and the energy $E$ for which we perform the calculation and is implicit in all Green's functions mentioned. We choose the energy $E$ with a small imaginary part $\eta$. This changes the Green's functions to retarded Green's functions.

The next step is to obtain or specify the Hamiltonian in matrix form of the individual unconnected slices. In other words we need $\mathbf{H}_{\text {leads }}$ and $\mathbf{H}_{n}$ for $n \in\{2,3, \ldots, N-1\}$, the Hamiltonian of the slices in the device. All these matrices are of size $W \times W$ in calculations done in this thesis.

In all the calculations in this thesis, $\mathbf{H}_{\text {leads }}$ is a matrix with $\left(\mathbf{H}_{\text {leads }}\right)_{i, i+1}=\left(\mathbf{H}_{\text {leads }}\right)_{i+1, i}=t$ and all other elements zero. $\mathbf{H}_{n}$ is specific for each model, but if no impurities or additional structure is imposed it is equal to the leads Hamiltonian matrix.

Next, we specify the hopping matrices between slices: $\mathbf{V}_{n, n+1}$ for $n \in\{1,2, \ldots, N-1\}$. This is sufficient as $\mathbf{V}_{n+1, n}=\mathbf{V}_{n, n+1}^{\dagger}$, following from the requirement that the Hamiltonian is Hermitian. The hopping in the leads and from the leads is chosen as $t \mathbf{1}$.

The next step is to compute the surface Green's function, $\mathbf{G}_{\text {surface }}$, from $\mathbf{H}_{\text {leads }}$ as was derived in section 3.4.2. For this routines exist to solve the eigenvalues and vectors of $\mathbf{H}_{\text {leads }}$. After completing this step the model may be thought of as $N+2$ slices where the first and last slice contain all the effects of the leads.

Because $\mathbf{g}_{n, n}^{-1}=E \mathbf{1}-\mathbf{H}_{n}$, we now have all the isolated Green's functions in our model. We also know all the connections we wish to add, $\mathbf{V}_{n, n+1}$. So now we may use the recursive Green's function equations (3.25) and (3.24) to connect all the slices

$$
\begin{aligned}
\mathbf{G}_{1, n+1}^{+} & =\mathbf{g}_{1, n}^{+} \mathbf{V}_{n, n+1} G_{n+1, n+1}^{+} \\
\mathbf{G}_{n+1, n+1}^{+} & =\left[\left(\mathbf{g}_{n+1, n+1}^{+}\right)^{-1}-\mathbf{V}_{n+1, n} \mathbf{g}_{n, n}^{+} \mathbf{V}_{n, n+1}\right]^{-1}
\end{aligned}
$$

This procedure starts with the surface Green's function, $\mathbf{g}_{1,1}^{+}=\mathbf{G}_{\text {surface }}$, and also ends with the surface Green's function, $\mathbf{g}_{N, N}^{+}=\mathbf{G}_{\text {surface }}$.

At the end of this procedure we have $\mathbf{G}_{1, N}^{+}$. We obtain $\mathbf{G}_{N, 1}^{-}$by taking the the hermitian conjugate of $\mathbf{G}_{1, N}^{+}$. We need the broadening function as specified in equation (3.16). We compute this by using the equation (3.17) for the self energy and inserting $\mathbf{V}_{L / R}=\mathbf{1} t$ and $\mathbf{g}_{L / R}^{+}=\mathbf{G}_{\text {surface }}$. So the broadening function is:

$$
\begin{equation*}
\boldsymbol{\Gamma}_{L / R}=i t^{2}\left(\mathbf{G}_{\text {surface }}-\mathbf{G}_{\text {surface }}^{\dagger}\right) \tag{3.36}
\end{equation*}
$$

With this, we finally have all the components required for the transmission function as specified in equation (3.14)

$$
T(E)=\operatorname{Tr}\left[\boldsymbol{\Gamma}_{L} \mathbf{G}_{1 N}^{+} \boldsymbol{\Gamma}_{R}\left(\mathbf{G}_{1 N}^{+}\right)^{\dagger}\right]
$$

Now we can compute the transmission. This we will do in the following chapters.

## Chapter 4

## Numerical Results Hofstadter Lattice

### 4.1 Perfect One-Dimensional Wire

The first model we describe is a perfect one-dimensional wire as introduced in equation (2.2), but with the chemical potential set to zero, $\mu=0$,

$$
\begin{equation*}
\hat{H}=\sum_{i} t \hat{c}_{i}^{\dagger} \hat{c}_{i+1}+t \hat{c}_{i+1}^{\dagger} \hat{c}_{i} \tag{4.1}
\end{equation*}
$$

We wish to find the transmission in this wire. For this we need to compute the retarded Green's function, $G_{1, N}^{+}(E)$, in the wire. We illustrate the lattice combined with the retarded Green's function we wish to find below:


For the purpose of calculating $G_{1, N}^{+}(E)$, we are not interested in the semi-infinite wires, only how they influence the Green's function on the sites 1 and $N$. So for calculations it is more useful to think of the semi-infinite leads as sites that have a different Green's function. So in the lattice representations we change the edges of semi-infinite leads to a single special site:


Thus we may think of the lattice as


The Green's functions of the edges of the semi-infinite wire was found in equation (3.34),

$$
\begin{equation*}
\bigotimes \Longrightarrow g_{1,1}(E)=g_{N, N}(E)=\frac{E-i \sqrt{4-\left(\frac{E}{t}\right)^{2}}}{2 t} \tag{4.2}
\end{equation*}
$$

### 4.1.1 Analytic Calculation

The perfect wire is simple enough to allow for an easy analytic calculation. This calculation is done to illuminate how a recursive algorithm works and check numerical results. We use the recursive Green's function formalism as derived in section 3.3 to obtain $G_{1, N}^{+}(E)$. We directly insert $V_{n, n+1}=V_{n+1, n}=t$ to obtain the a simplified set of recursive equations

$$
\begin{align*}
G_{n+1, n+1} & =\left(g_{n+1, n+1}^{-1}-t^{2} g_{n, n}\right)^{-1}  \tag{4.3}\\
G_{1, n+1} & =t g_{1, n} G_{n+1, n+1} \tag{4.4}
\end{align*}
$$

We start the recursive equations with the surface Green's function, as derived in equation (3.34)

$$
\begin{equation*}
t g_{1,1}=t g_{\text {surface }}=\omega-i \sqrt{1-\omega^{2}} \tag{4.5}
\end{equation*}
$$

where $\omega=E /(2 t)$. For the first $N-2$ iterations of the recursive Green's function method, $g_{n+1, n+1}^{-1}=E$ and the surface Green's function remains identical, $G_{n, n}=g_{\text {surface }}$. This is expected, as $g_{\text {surface }}$ was defined as the Green's function that remains identical under extension with a slice. Thus equation (4.4) may be rewritten to

$$
\begin{equation*}
G_{1, n+1}=t g_{1, n} g_{\text {surface }} \tag{4.6}
\end{equation*}
$$

Using this we write the Green's function for the chain, connected up until site $N-1$, as

$$
\begin{equation*}
t g_{1, N-1}=\left(\omega-i \sqrt{1-\omega^{2}}\right)^{N-1} \tag{4.7}
\end{equation*}
$$

The absolute value of $g_{1, N-1}$ is identical to that of the Green's function we started with $g_{1,1}$, because $\omega-i \sqrt{1-\omega^{2}}$ only contains a phase if $\omega \leq 1$.

For the last step of the recursive algorithm, connecting site $N$ we have $g_{n+1, n+1}^{-1}=t\left(\omega+i \sqrt{1-\omega^{2}}\right)$. Thus $G_{N, N}$ is:

$$
\begin{equation*}
t G_{N, N}=\frac{1}{2 i \sqrt{1-\omega^{2}}} \tag{4.8}
\end{equation*}
$$

So $G_{1, N}$ is

$$
\begin{equation*}
t G_{1, N}=\frac{\left(\omega-i \sqrt{1-\omega^{2}}\right)^{N-1}}{2 i \sqrt{1-\omega^{2}}} \tag{4.9}
\end{equation*}
$$

To calculate the transmission we also need the broadening functions. The expression for the broadening function follows from the surface Green's function of equation (4.5) and the definition of the broadening function equation (3.16)

$$
\Gamma_{L}=\Gamma_{R}= \begin{cases}2 t \sqrt{1-\omega^{2}}, & |\omega|<1  \tag{4.10}\\ 0, & \text { else }\end{cases}
$$

Consequently $\Gamma_{L} G_{1, N}$ is a phase if $|\omega|<1$ and zero otherwise. The phase cancels against its complex conjugate, $\Gamma_{R} G_{1, N}^{\dagger}$. Therefore the transmission of a perfect one dimensional wire is

$$
T(E)=\Gamma_{L} G_{1, N} \Gamma_{R} G_{1, N}^{\dagger}= \begin{cases}1, & |E / 2 t|<1  \tag{4.11}\\ 0, & \text { else }\end{cases}
$$

### 4.1.2 Green's Functions Cut-off Dependence

In the numerical calculations the retarded Green's function $G_{1, N}^{+}$is calculated. The retarded Green's function is related to the Green's function by a shift in energy with an infinitesimal imaginary number, $G_{1, N}^{+}(E)=\lim _{\eta \rightarrow 0} G_{1, N}(E+i \eta)$. The limit of $\eta$ going to zero, is implemented in numerical calculations by
choosing $\eta$ to be small but finite.
To develop an understanding of the effects of $\eta$ on numerical results, it's effects on the Green's function in the perfect one-dimensional wire are studied. This has as advantages that all objects are scalars and we have analytical results.
The Green's functions are computed numerically using the recursive Green's function method. The results


Figure 4.1: The Green's function, $t G_{1,10}$, with $\eta=0.001$. The real component is shown in blue, The imaginary component is shown in red and the absolute value is shown in Green.
of the calculation are shown in figure 4.1 for a system of 10 sites. The real and imaginary components of the Green's function fluctuate, but the absolute value behaves as $1 /\left(\sqrt{1-(E / t)^{2}}\right)$. The fluctuations increase proportionately for larger systems. The divergences at $E / t= \pm 2$ show why it is necessary to include a imaginary part $\eta$ in the numerical calculations.

A more detailed study of the behaviour of the Green's function at fixed energy as a function of $\eta$ is shown in figure 4.2. At the energy, $E / t=1$, the Green's function, $G_{1, N}^{+}$, increases as we decrease $\eta$. This makes the inclusion of $\eta$ necessary as the Green's function is undefined at this energy otherwise. For energy's not subject to divergences such as: $E / t=0$ and $E / t=1.8$, the Green's function is independent of $\eta$ when $\eta$ is smaller than $10^{-2}$. Consequently numerical results are independent of $\eta$ when $\eta$ is sufficiently small.


Figure 4.2: Behaviour of the absolute value of $t G_{1,10}$ depending on the imaginary shift of the energy, $\eta$. We show show this behaviour for three values of energy: The blue line is for $E / t=2$, the red line is for $E / t=1.9$ and the green line is for $E / t=0$.

### 4.1.3 Impurity Effects

By choosing a non-trivial profile the local chemical potential, $\mu_{i}$, the effects of impurities are investigated. For this three different models are studied, for which we show the transmission results in figure 4.4.

The first model is that of the perfect one-dimensional wire, where there is no local chemical potential, $\mu_{i}=0$. The results for this model match the prediction of equation (4.11), where we have perfect transmission when inside the region where modes exist and zero outside. A further note is that this result is independent of the amount of sites, as we would expect from physical grounds.


Figure 4.3: A sketch of a one-dimensional wire with an impurity on the 5th site.

The second model is that of a single impurity. A sketch of this model is shown in figure 4.3. For this model the chemical potential is zero, $\mu_{i}=0$, except for a single site, $\mu_{5}=t$. For this model we obtain a reduced conductivity, where the amount of the reduction depends on the strength of the impurity. This result is in agreement with earlier work [26]. The transmission results of a single impurity does not depend on the location of the impurity or the chain length.

The last model is that of random impurities at all of the 8 sites. In this model we assign a random number to the chemical potential at each site, $\mu_{i} \in[-t, t]$. This model is used to describe disorder on the lattice. For longer chains the transmission decreases further and becomes courser.


Figure 4.4: Transmission for three different chains of 10 sites, with $\eta=10^{-8}$. The Blue line is for a chain without impurity's. The red line has a single impurity at the 5 th site. The green line has random impurity's located in the 8 sites in-between the edge sites.

### 4.2 Finite Width Wire

In the previous section the results for a wire with width $W=1$ where discussed. This section establishes the behaviour of wires with widths larger than one, $W>1$.

First we show the results for a wire with a width, $W=3$, in figure 4.5. The transmission looks as a pyramid centred around $E=0$. This feature repeats in larger width wires as may be seen in figure 4.6.

The pyramid like structure originates from having multiple bands of perfect transmission stacked on


Figure 4.5: The transmission trough a wire with width, $W=3$.
each other. This is because all individual slices in the model have an identical Hamiltonian

$$
\mathbf{H}_{\text {slice }}=\left(\begin{array}{ccc}
0 & t & 0  \tag{4.12}\\
t & 0 & t \\
0 & t & 0
\end{array}\right)
$$

We can diagonalize this matrix,

$$
\begin{equation*}
\mathbf{S}^{\dagger} \mathbf{H}_{\text {slice }} \mathbf{S}=\operatorname{diag}\left(E_{1}, E_{2}, E_{3}\right)=\operatorname{diag}(-\sqrt{2} t, 0, \sqrt{2} t) \tag{4.13}
\end{equation*}
$$

As the surface Green's functions, $\mathbf{g}_{\text {surface }}$, and hopping matrices, $\mathbf{V}_{n, n+1}$, are diagonal in the same basis, all matrices in the recursive Green's function formalism are diagonal. This leads to the model being effectively a superposition of wires of width one, but with energy's shifted by $E_{w}$.

Thus in the transmission we have a superposition of perfect transmission intervals, centred around $E_{w}$, with perfect transmission between $E_{w}-2 t$ to $E_{w}+2 t$. This allows us to explain the pyramid structure of figure 4.5 , where we have $E_{w}=\{-\sqrt{2} t, 0, \sqrt{2} t\}$.


Figure 4.6: The transmission divided by the width $W$ of the wire. We plot multiple wires with widths: $W=9, W=27, W=81$.

For wider chains the energy's, $E_{w}$, are be found by identifying a slice of width $W$ with a one-dimensional wire with a length of $L=W$. The solutions of open one-dimensional chains are given by sinusoids, $\Psi_{w}(x) \sim$ $\sin \left(\kappa_{w} x\right)$, where $\kappa_{w}=\pi w /(W+1)$. This choice ensures that the wave-function is zero on points outside of the chain, $\Psi_{w}(0)=\Psi_{w}(W+1)=0$. The energies of these solutions are [26]

$$
\begin{equation*}
E_{w}=2 t \cos \left(\kappa_{w}\right) \tag{4.14}
\end{equation*}
$$

The smallest energy $E_{w}$ is $-2 t \cos \left(\frac{\pi}{W+1}\right)$ and the largest $E_{w}$ is $-2 t \cos \left(\frac{\pi}{W+1}\right)$. As the width is taken to infinity, $W \rightarrow \infty$, the maximum energy and minimum energy converge to $2 t$ and $-2 t$ respectively. Combining this with the width of a single transmission interval, it follows that, in the limit of $W \rightarrow \infty$, all transmission lies between $-4 t$ and $4 t$.

The results of figure 4.6 suggest that $T(E=0) \sim W$ and that the overall form converges for $W \rightarrow \infty$.
In figure 4.7 we compute the transmission for a devices similar to the finite width $W$ wires we discussed earlier, but now we give each site inside the device a random chemical potential, $\mu_{i} \in[-\zeta, \zeta]$.


Figure 4.7: The transmission for a wire of width $W=27$ and length $L=27$. The results for four different strengths of the random potential, $\zeta$, are shown.

### 4.3 Magnetic Field Implementation

We want to study the effects of a magnetic field in both the square lattice model and the Sierpinski carpet. In this section we show how a magnetic field is implemented in a square lattice. The common way of introducing a magnetic field in a tight-binding model is by using Peierls substitution [22, 27]. We gave a sketch of how this substitution works in section 2.3 .2 , but rigorous work to justify this substitution may be found [28, 29, 30]. The Peierls substitution changes the hopping element between two lattice points $i$ and $j$ with a phase. This phase depends on the gauge field between the lattice points,

$$
\begin{equation*}
t_{i, j} \rightarrow t_{i, j} \exp \left(\frac{-i e}{\hbar} \int_{\vec{x}_{i}}^{\vec{x}_{j}} \vec{A} \cdot d \vec{x}\right) \tag{4.15}
\end{equation*}
$$

Equation (4.15) summarizes how one implements the magnetic field on the lattice, but to provide more physical understanding we derive the same result from the Aharonov-Bohm effect [31]. The Aharonov-Bohm effect states that a charged particle obtains a phase shift, $e^{i \phi}$, when it loops around an area with non-zero magnetic field inside, even if there is no magnetic field on the path. The phase, $\phi$, the charged particle acquires is

$$
\begin{equation*}
\phi=\frac{q}{\hbar} \int_{\mathrm{C}} \vec{A} \cdot d \vec{x}, \tag{4.16}
\end{equation*}
$$

where $q$ is the electric charge of the particle and C is closed path of the particle. If the magnetic field is constant, then this expression may be simplified to

$$
\begin{equation*}
\phi=\frac{q}{\hbar} A(\mathrm{C}) B \tag{4.17}
\end{equation*}
$$

by using $\vec{B}=\nabla \times \vec{A}$ and stokes theorem. Here $A(\mathrm{C})$ is the area enclosed by the path C.
To show how the Aharonov-Bohm effect translates into the tight-binding model, we begin by studying the effects of the magnetic field on a single plaquette. We illustrate a plaquette in figure 4.8. In this model the electron is restricted to moving from one lattice site to a different site, thus by going around a loop in the plaquette it encloses a flux, $\Phi=A(\mathrm{C}) B=a^{2} B$. Here $a$ is the distance between two lattice points.


Figure 4.8: a plaquette in a magnetic field. The arrows represent an electron hopping a closed loop through the chain.

An electron going around a loop in this plaquette must obtain a phase trough the hopping elements,

$$
\begin{equation*}
t_{1} t_{2} t_{3}^{\dagger} t_{4}^{\dagger}=t^{4} e^{-i 2 \pi \Phi / \Phi_{0}} \tag{4.18}
\end{equation*}
$$

where $\Phi_{0}=2 \pi \frac{h}{e}$. For a single plaquette it is sufficient that one hopping element contains a phase $t_{3}=$ $t e^{i 2 \pi \Phi / \Phi_{0}}$ and all other hopping are real. However, we wish to describe a lattice with multiple plaquettes in a magnetic field. If the magnetic field is constant, then each plaquette in the lattice encloses the same amount of flux, as visualised in figure 4.9. To implement this one must choose the hopping elements such


Figure 4.9: An example of a two dimensional square lattice structure, with a constant magnetic field inbetween the leads.
that for any closed paths the obtained phase trough the hopping elements corresponds to the flux enclosed in the path. This is true if one picks the Landau gauge $\vec{A}=-B y \hat{x}$. This gives the hopping elements in the $x$ direction a phase depending on the $y$ position of the hopping,

$$
\begin{equation*}
t_{x}=t \exp \left(i 2 \pi \Phi / \Phi_{0} I_{y}\right) \tag{4.19}
\end{equation*}
$$

where $I_{y}$ is an index in the $y$ direction. This index is chosen such that $a I_{y}$ is the position in the $y$ direction of the two lattice points that participate in the hopping. The hopping in the $y$ direction is unaffected, $t_{y}=t$. This choice of hopping ensures that for any closed path the phase acquired matches the Aharonov-Bohm effect.

### 4.4 The Hofstadter Model

By using the prescription given in the previous section, the effects of the magnetic field may be studied. In the left panel of figure 4.10 the transmission as a function of energy, $E / t$, and magnetic field, $\Phi / \Phi_{0}$, are shown. In the results of figure 4.10 similarity with the Hofstadter butterfly may be seen [8]. This is because the model in-between the leads is the Hofstadter model, but with a major difference. Namely our model has edges and the Hofstadter model does not. In the following sections we further investigate the correspondence between our results and the Hofstadter butterfly.


Figure 4.10: Transmission results for a Hofstadter model with a width of $W=81$ and length $L=81$. The arrows point to plateaus where the transmission is: one, two or three.

### 4.4.1 Bulk Modes

It is possible to compute the transmission as shown in figure 4.10 for different sizes of the lattice. This allows us to compare how the results change for different system sizes $W$ and $L$. For these comparisons we choose to fix the size of the lattice between the leads to a square, so $W=L$. We make this choice such that, the scaling we investigate here is the same as for the Sierpinski carpet. To investigate how transmission changes we introduce a new function $\Delta T$ that is the difference in transmission between a large square and a smaller square,

$$
\begin{equation*}
\Delta T=T(W=81, L=81)-T(W=27, L=27) \tag{4.20}
\end{equation*}
$$

$\Delta T$ is computed for a mesh of energy and flux values, these results are shown in figure 4.11. By subtracting the results of a smaller system, we subtracted any effects that are independent of the system size. We refer to the states in areas that do not increase in transmission as edge modes for reasons that will become apparent in section 4.4.4. The states in areas that increase in transmission as the system size increases are referred to as bulk modes.


Figure 4.11: Left: $\Delta T$ as defined in equation (4.20). Right: The spectrum of solutions for the Hofstadter model as computed by [8].

In figure 4.11 we also show the Hofstadter butterfly. The Hofstadter butterfly is the spectrum of solutions for an infinite 2 d lattice with a magnetic field. To be more precise it shows if there exists a solution $\psi(x, y)$ for the equation

$$
\begin{aligned}
& t\left[\psi(x+a, y)+\psi(x-a, y)+\left(e^{i 2 \pi\left(\Phi / \Phi_{0}\right)}\right)^{(x / a)} \psi(x, y+a)\right. \\
& \left.\quad+\left(e^{-i 2 \pi\left(\Phi / \Phi_{0}\right)}\right)^{(x / a)} \psi(x, y-a)\right]=E \psi(x, y)
\end{aligned}
$$

for a specific energy, $E / t$, and a specific flux, $\Phi / \Phi_{0}$. Analytic solutions only exist when $\Phi / \Phi_{0}$ is a rational number. This confused scientist as no other physical effects depend on being able to express a physical quantity as a rational number. Hofstadter showed in 1976 that the spectrum is in fact continuous in terms of the magnetic field.

The model that Hofstadter solved is equal to the model that is used in this thesis, with the mayor exception that the lattice in this thesis is finite and is coupled to semi-infinite leads. Reassuringly, we observe that the results of Hofstadter and $\Delta T$ largely agree. This agreements is desired as Hofstadter's results describe the density of states in the limit of $W \rightarrow \infty$ and $L \rightarrow \infty$, with the exception of states that exist on the boundary.

A noticeable difference is that there are lines in Hofstadter's results near $\left(\Phi / \Phi_{0}=0, E / t=-4\right)$ that are absent in the results of $\Delta T$. The reason for this is that as these lines approach $\left(\Phi / \Phi_{0}=0, E / t=-4\right)$ they become very thin. This is the reason why they do not show up in numerical results. In the results of figure 4.13 we further confirm that these modes become thinly spaced for small magnetic field.

### 4.4.2 Direct Diagonalization

To supplement our understanding of features we may directly diagonalize the Hamiltonian. To do this we construct the Hamiltonian matrix, $\mathbf{H}$, of the system without the leads connected for a fixed flux. This means that $\mathbf{H}$ is a large, but finite, matrix.

Because $\mathbf{H}$ is finite, we may solve for the eigenvalues of $\mathbf{H} \vec{\psi}_{n}=E_{n} \vec{\psi}_{n}$. This provides us with as many states, $\vec{\psi}_{n}$, as there are lattice points. For example for the results of figure 4.10 has $81^{2}=6561$ states.

From the eigenvectors, $\vec{\psi}_{n}$, we are interested in the localization of the state on the lattice. To show this we display $\left|\psi_{n}(x, y)\right|^{2}$. An example of this for a square lattice is shown in figure 4.12. Here a few examples where chosen to illustrate how bulk states are localized. For a small energy range inside a bulk region many different bulk states exist, although they are quite different from each other, they are generally localized throughout the entire lattice.


Figure 4.12: Examples of states in bulk regions. The states were obtained by directly diagonalising a Hamiltonian with flux $\Phi / \Phi_{0}=0.27$. The arrows refer to the energy of the state in the transmission graph that is obtained by the recursive Green's formalism. The black line shows where in the Hofstadter butterfly the intersection at flux $\Phi / \Phi_{0}=0.27$ lies.

By directly diagonalising a Hamiltonian for a specific flux value, we also obtain the list of energy eigenvalues $E_{n}$ for the system. This allows us to show the density of states. We do this by making a histogram with a very small bin size. We show two such histograms for fluxes of $\Phi / \Phi_{0}=0.11$ and $\Phi / \Phi_{0}=0.22$ in figure 4.13. Almost all the bins contain at least one state, these are the edge modes and they exist for the entire spectrum.

The peaks in the histograms correspond to the bulk modes. In both histograms the outermost peaks correspond to the same line in the Hofstadter butterfly. So we may investigate the difference between them in the two histograms. This outermost peak changes from multiple bins when the flux is $\Phi / \Phi_{0}=0.22$ to a single bin $\Phi / \Phi_{0}=0.11$. Thus reinforcing the claim that these bulk modes become thin as one approaches $\left(\Phi / \Phi_{0}=0, E / t=-4\right)$.


Figure 4.13: Left: A histogram of the states per energy for a flux of $\Phi / \Phi_{0}=0.11$. Right: A histogram of the states per energy for a flux of $\Phi / \Phi_{0}=0.22$. Both histograms are for a system of width, $W=81$, and size, $L=81$, and therefore contain 6561 states. The bins in both histograms have a width of $1 / 100$ in units of $E / t$.

### 4.4.3 Landau Levels

In section 2.3.1 we found that we could identify the tight-binding model as a discretized version of the free electron model. This connection is only valid if the discretization is sufficiently small that the effects of the lattice are negligible. This condition is true if the energy of the modes is small, as then the wavelength of the modes is appropriately large. We use this connection to show how the integer quantum Hall effect translates to our transmission results.

The starting point for this correspondence is to find how the energies of the Landau levels translate to tight-binding parameters. As derived in section 2.4, the energy of the $n$-th Landau level is

$$
\begin{equation*}
E_{n}=\hbar \omega_{B}\left(n+\frac{1}{2}\right) \tag{4.21}
\end{equation*}
$$

where $\omega_{B}=e B / m$. In section 2.3.1 we derived how $t$ relates to $a$ and $m$. Namely: $t=-\hbar^{2} /\left(2 m a^{2}\right)$. This allows us to write the energy of the Landau levels to

$$
\begin{equation*}
E_{n}=4 \pi t \frac{\Phi}{\Phi_{0}}\left(n+\frac{1}{2}\right)-4 t . \tag{4.22}
\end{equation*}
$$

The factor of $-4 t$ arises from the global chemical potential, $\mu$. As the global chemical potential obtains a factor of $-2 t$ per dimension during the discretization. We combine the Landau levels with the transmission in figure 4.14.

The Landau levels themselves do not show up in transmission spectrum, but the lack of these lines was already noted in the result of figure 4.11 . However, the Landau levels do correspond with a change of the transmission with an integer value.

One of the predictions of the integer quantum Hall effect is that each filled Landau level contributes a factor of $e^{2} / h$ to the Hall conductance, $\sigma_{x y}$. In terms of transmission functions this means that the transmission is the amount of filled Landau levels. This is what we see in figure 4.14.

A small problem is: we are are not measuring the Hall conductance, $\sigma_{x y}$, but the cross-sample conductance, $\sigma_{x x}$. The reason this result shows up in the cross-ample conductance, is because the Hall conductance is caused by chiral edge modes. The presence of the chiral edge modes creates perfect channels around the edges, this gives rise to the Hall conductance, $\sigma_{x y}$. But these same channels allow electrons to move from the left edge to the right edge, thus giving rise to the same conductance for $\sigma_{x x}$.


Figure 4.14: Transmission results for width $W=81$ and length $L=81$ combined with the prediction of Landau levels of equation 4.22, where we show the $n$-th Landau level, with $n \in\{0,1,2,3,4\}$.

### 4.4.4 Chiral Edge Modes

In the previous section the connection with the integer quantum Hall effect was established. This allows us to identify that plateaus of integer transmission are generated by chiral edge modes, at least for the domain where the connection with the free electron model holds. In this section we establish the connection between chiral edge modes and the integer plateaus in the entire flux energy domain.

Similar to the integer quantum Hall effect, it is found that for the Hofstadter model the Hall conductance is quantized

$$
\begin{equation*}
\sigma_{x y}=\frac{e^{2}}{h} \mathcal{C} \tag{4.23}
\end{equation*}
$$

but instead of the amount of filled Landau levels, the quantization is determined by the first Chern number, $\mathcal{C}$ [18]. The first Chern number is an integer number that is based on a momentum integral over the filled bands. In the integer quantum Hall effect one finds that each Landau level contributes exactly one to the Chern number. However, in general the contribution of each band can be any integer. An important property of the Chern number is that it only changes when the distinction between empty bands and filled bands breaks down. In other words, if the gap between the bands closes and the bulk of the system becomes conducting.

If the Chern number is only defined when the system is insulating, then how does the system obtain a Hall response as equation (4.23) suggests? This is because the calculation for the Chern number relied on an infinite system, without boundary. But a real system terminates at some point. This does not invalidate the Chern number calculation, as for a sufficiently large system, the inner or bulk regions may be described by an infinite model, but it does break down at the boundary. At this boundary there are states that have properties that directly relate to the Chern number, this is called the Bulk-boundary correspondence [20]. For the Hofstadter model one finds that the edge of the lattice there are chiral edge modes. Where the the amount and the chirality of chiral edge modes is directly related to the Chern number in the bulk [32, 33].

The chiral modes allow us to explain the plateaus in the transmission. For if we compare our results to literature that directly computes $\sigma_{x y}$ [34], We observe that our results, $\sigma_{x x}$, are the approximately the absolute value of the expected Hall conductance, $\sigma_{x x} \approx\left|\sigma_{x y}\right|$. We show this comparison in figure 4.15. This makes sense, as the transmission from the left lead to the right only relies on the presence of a perfect channel, not it's chirality.


Figure 4.15: Left: Transmission results for recursive algorithm for a region of width $W=81$ and length $L=81$, with a linear scale for the transmission. Right: Hall conductance as computed by [34]. The darker colours refer to lower Hall conductance.

When we investigate the Sierpinski carpet, there is no literature that provides us with a connection to Chern numbers, thus to be able to verify that there are chiral edge modes, we have to rely on numerical results. There are multiple properties that chiral edge modes exhibit that we can check. These are: Resistance to impurities, being localized on the edge, integer transmission values and that the transmission remains constant across different system sizes. We investigate these properties in the Hofstadter model to build up familiarity with these results.

We begin by investigating the localization of the states in the regions that contain chiral edge modes. Examples of the states in the plateaus are shown in figure 4.16 . We find that these regions only contain modes that are heavily localized on the edges.


Figure 4.16: Up: Examples of the localization of edge states. Down left: A slice trough flux $\Phi / \Phi_{0}=0.11$, with examples of states at $E / t=\{-3,-2,-1\}$. Down right: transmission results for square lattice model with $W=81$ and length $L=81$. The black line is the location of the slice trough flux $\Phi / \Phi_{0}=0.11$. The dots refer to the examples of localization: $\left(\Phi / \Phi_{0}=0.27, E / t=0.3\right),\left(\Phi / \Phi_{0}=0.27, E / t=0.5\right)$ and $\left(\Phi / \Phi_{0}=0.48, E / t=0.3\right)$.

The other point of investigation is to verify that the transmission in the regions containing chiral edge modes is stable to impurities. We may check this by adding random impurities trough the local chemical potential, $\mu_{i} \in[-0.3 t, 0.3 t]$. By repeating the calculation of the transmission 40 times for the same energy and flux, we obtain an average transmission, $T_{A}$, and the standard deviation, $\sigma$.

This calculation is done for a mesh of energy and flux values and we show the result in figure 4.17. The edge mode regions have a standard deviation that is significantly smaller than the bulk regions. Furthermore the results of the standard deviation do show lines where we expect the Landau levels to be. This happens because impurities cause a broadening of the spectrum.


Figure 4.17: The results for calculations with random impurities, $\mu_{i} \in[-0.3 t, 0.3 t]$, generated by 40 samples for a hofstadter model with width,$W=27$ and size, $L=27$. Left: Average transmission, $T_{A}$. Right: Standard deviation, $\sigma$.

### 4.4.5 Symmetries

In the results of the Hofstadter butterfly there are two axis of reflection: a horizontal axis for $E / t=0$ and a vertical axis for $\Phi / \Phi_{0}=1 / 2$. These symmetries originate from the Hofstadter model, which we prove in this section. The presence of these symmetries implies that only a quarter of points in the transmission results is unique.

To prove the symmetry trough the $E / t=0$ axis, we will prove that the spectrum of solutions is symmetric around $E / t$. To this end, we introduce the flip operator, $\hat{F}$. The flip operator acts on a state $\psi(j, k)$ by multiplying with -1 in a checker-board manner

$$
\begin{equation*}
\hat{F} \psi(j, k)=(-1)^{j+k} \psi(j, k) \tag{4.24}
\end{equation*}
$$

We want to find how the flip operator changes the energies of solutions to the original problem, $\hat{H} \psi_{n}=E_{n} \psi_{n}$. From the original wave-function a modified wave-function, $\psi_{n}^{\prime}$, is obtained by applying the flip operator to the original wave-function, $\psi_{n}^{\prime}=\hat{F} \psi_{n}$. Then we compute the energy of this modified wave-function

$$
\begin{aligned}
\hat{H} \psi_{n}^{\prime} & =\hat{H} \hat{F} \psi_{n} \\
& =\hat{F} \hat{H}^{\prime} \psi_{n}
\end{aligned}
$$

where we introduce a modified Hamiltonian, $\hat{H}^{\prime}=\hat{F} \hat{H} \hat{F}$. Because of the square lattice structure, the modified Hamiltonian acts as if the hopping parameter sign was reversed, $\hat{H}^{\prime}=\hat{H}(t \rightarrow-t)$. If the chemical potential is zero, which is true for most models in this thesis, the modified Hamiltonian is the negative of the original Hamiltonian, $\hat{H}^{\prime}=-\hat{H}$. We apply this relation to find that the energy of the modified wave-function is minus the energy of the original wave-function. Thus, every solution $\psi_{n}$ with energy $E_{n}$ has a 'sibling solution' $\hat{F} \psi_{n}$ with energy $-E_{n}$. This relation generates the axis of symmetry trough $E=0$.

The symmetry trough $\Phi / \Phi_{0}=1 / 2$ is caused by a combination of two different symmetries. The first symmetry is that the the model is invariant under the addition of an integer of flux, $\Phi / \Phi_{0} \rightarrow \Phi / \Phi_{0}+n$. As the flux only influences the phase-factors and these are invariant under additions of integers, $e^{-i 2 \pi \Phi / \Phi_{0}}=$ $e^{-i 2 \pi\left(\Phi / \Phi_{0}+n\right)}$. The second symmetry is the invariance of the energy spectrum under complex conjugation of the Hamiltonian. Complex conjugation changes the the phase factors by $e^{-i 2 \pi \Phi / \Phi_{0}} \rightarrow e^{+i 2 \pi \Phi / \Phi_{0}}$. This is equivalent to reversing the magnetic field, $B \rightarrow-B$.

To prove that the energy spectrum is invariant under a reversed magnetic field, we repeat the previous calculation, but with the conjugation operator, $\hat{C}$. The Hamiltonian, $\hat{H}$, with magnetic field $B$ is related to $\hat{H}^{*}$ with magnetic field $-B$ by $\hat{H}^{*}=\hat{C} \hat{H} \hat{C}$. Assuming we have a solution $\hat{H} \psi_{n}=E_{n} \psi_{n}$, then we introduce $\psi_{n}^{*}=\hat{C} \psi_{n}$. This modified wave-function is a solution of the same problem, but with magnetic field reversed, and with the same energy $E_{n}$

$$
\begin{aligned}
\hat{H}^{*} \psi_{n}^{*} & =\hat{C} \hat{H} \psi_{n} \\
& =E_{n} \psi_{n}^{*}
\end{aligned}
$$

So we have two symmetries for the spectrum: $\Phi / \Phi_{0} \equiv \Phi / \Phi_{0}+n$ and $\Phi / \Phi_{0} \equiv-\Phi / \Phi_{0}$. By combining the two symmetries we obtain a new symmetry

$$
\begin{equation*}
\Phi / \Phi_{0} \equiv 1-\Phi / \Phi_{0} \tag{4.25}
\end{equation*}
$$

This symmetry responsible for the axis of reflection trough $\Phi / \Phi_{0}=1 / 2$.

### 4.4.6 Conclusion

We close the discussion on the Hofstadter model by reiterating the division into chiral edge and bulk mode regions. We showed that the chiral edge modes are localized on the edges and the transmission they generate is resistant to impurities. In contrast the bulk modes are localized through the entire lattice and the transmission they generate is easily influenced by impurities. By investigating the scaling of the transmission we can nicely show where both are located in the flux energy space. For this we define the scaling function, $S$, as the transmission through a large Hofstadter model divided by the transmission through a small Hofstadter model,

$$
\begin{equation*}
S=\frac{T(W=81, L=81)}{T(W=27, L=27)} \tag{4.26}
\end{equation*}
$$



Figure 4.18: The scale function, $S$, as defined in equation (4.26).

We display the results of $S$ in figure 4.18. The white areas are where the transmission is close to zero and were manually put to zero. The purple areas correspond to non-zero transmission and that the transmission remains identical when changing the system size, these are also the areas where we find chiral edge modes. We expect that the scaling is unity for regions containing chiral edge modes, as the amount of transmission channels is fixed by the Chern number, not the system size.

The remaining areas increase in transmission as the system size increases. These areas correspond to the areas where we observed the bulk modes. The maximum scale factor observed, barring the region near $\Phi / \Phi_{0}=1 / 2$, is 3 . This is desired as the width was increased by 3 , so we would expect the amount of channels participating in the transmission to increase with the same factor as the width.

## Chapter 5

## Numerical Results Sierpinski Carpet

### 5.1 Sierpinski Lattice Model

We started chapter 1 with explaining what fractals are and why they are interesting to study. Fractals are objects that have a non-integer dimension when dimension is defined through scaling properties. The fractal we study is the Sierpinski carpet. The main reason for this choice is that it translates naturally into the recursive green's function equations.

A Sierpinski carpet is a fractal structure generated by taking a square, dividing the square into 9 pieces, removing the square in the center and repeating the procedure for the 8 remaining squares. In figure 5.1 we show the different iterations of this procedure.


Figure 5.1: The first four generations of the Sierpinski carpet. The generation corrosponds to how often the recursive procedure for generating the fractal was applied.

The recipe for the creation of the Sierpinski carpet also provides us with the method for finding the fractal dimension. As decreasing the length scale by a factor of three, $l \rightarrow l^{\prime}=l / 3$, increases the amount of filled boxes by a factor of eight, $N(l) \rightarrow N(l / 3)=8 N(l)$. So we find that $N(l) \sim(1 / l)^{8 / 3}$. Using the definition of box dimension we find

$$
\begin{equation*}
d_{\text {box }}=\lim _{l \rightarrow 0} \frac{\log (N(l))}{-\log (l)}=\frac{\log (8)}{\log (3)} \approx 1.8928 . \tag{5.1}
\end{equation*}
$$

We implement the Sierpinski carpet into the Hofstadter model, by starting with a square lattice with the width and length being a power of three: $W=L=3^{G}$, where $G$ is the generation of the fractal we wish to make. Then we divide the lattice into 9 blocks and remove any lattice points in the center block. This is repeated until the final blocks contain only a single lattice point. An illustration of how the lattice of a generation two carpet looks is shown in figure 5.2.


Figure 5.2: The implementation of the Sierpinski carpet into the tight-binding model.

### 5.2 Sierpinski Lattice without Magnetic Field



Figure 5.3: Transmission results of a Sierpinski carpet of generation 4. Localization of a few example states are shown, with arrows referring to their approximate energy.

By using the recursive Green's function formalism we obtain the transmission spectrum for a Sierpinski fractal. This spectrum is shown in figure 5.3. There are a few things to note about this spectrum. First, we observe a lot of fluctuations over the depicted energy range. These fluctuations have been studied in the past [6], where it was found by using box-counting that these fluctuations have a fractal behaviour. Specifically, the fluctuations scale with the same dimension as the fractal, i.e. $d \approx 1.89$.

Nonetheless there exists a small domain which is flat. This domain is located near $E=0$, where the transmission is approximately four. Another fascinating property of this region is that the states obtained by direct diagonalization have the shape of a simple cross and a square as shown in figure 5.3. This feature persists across different generations of the Sierpinski carpet.

A striking difference with the simple two-dimensional lattice is that the transmission value is small compared to the system size. For the two-dimensional lattice with a width of $W$ we obtained a transmission maximum that was proportional to the width, whereas here, ignoring minor fluctuations the transmission maximum is four. For the two-dimensional lattice one can think of this as the transmission maximum being proportional to the amount of horizontal lines through which a particle can travel, i.e. the width. A major difference with the Sierpinski carpet is that when holes are cut out, the amount of horizontal channels is reduced. However,
even the slice with the fewest points still has $2^{G}$ points, so for the result shown figure 5.3 we naively would expect a maximum transmission of $2^{4}=16$, but we only observe a maximum slightly above four instead.

### 5.3 Magnetic Field Results

The introduction of the magnetic field does not require additional steps in comparison to the Hofstadter, as the implementation of the magnetic field as done in section 4.3 ensures that for larger paths the appropriate phase is obtained. The results of computing the transmission for the Sierpinski carpet of generation four are shown in figure 5.4.

In sharp contrast to the results without magnetic filed, where almost the entire spectrum contains fluctuations, there are large domains where the transmission is close to one. As we will prove in section 5.3.2, these domains contain chiral edge modes. But there are more domains that have integer transmission. Around $\left(\Phi / \Phi_{0}=1 / 2, E / t=0\right)$ there is an area of transmission two. In this area we find non-chiral edge modes. Section 5.3.3 is devoted to a further discussion of this feature.

In the transmission results without magnetic field of figure 5.3 , a small plateau of transmission four was visible near $E=0$. We observe that this plateau extends to finite magnetic field in the results of figure 5.4. This plateau remains present in different generations. One may verify this by comparing the results of different generations, as done in figure 5.9.


Figure 5.4: Transmission for the Sierpinski carpet of generation, $G=4$, with a width of: $W=81$ and Length: $L=81$.

Next we investigate the transmission results for different generations of the Sierpinski carpet. If features persist across different generations, we can assume that this is true for all generations and not just the few accessible. We show the results for generation 3 and generation 5 in figure 5.5. The same colour-scale was
used for all generations. We are able to do this because the transmission rarely exceeds four, regardless of generation. Comparing these results shows that large scale features for generations 3,4 and 5 remain mostly identical, with a major exception being the coarse graining for domains not part of a plateau.

The increase in coarseness for larger generations is likely caused by the self-similarity of the spectrum. As for the Sierpinski triangle it is known that each successive generation adds more small scale structure to the spectrum [35]. Section 4.4.1 is devoted to studying the areas that show this increase in coarseness.

Although we have transmission results for generation 5, we chose to rely mainly on generation 4 results. This is due to the computational time necessary to compute the transmission for a generation 5 Sierpinski carpet, but this is compounded by the presence of small scale structure. As to capture the small scale structure more and more sampling is required, otherwise the transmission value chosen to represent the area under the pixel contains a high degree of randomness. The increase of sampling required combined with the increase of computational time for a single transmission result, motivates the choice predominately use the generation 4 results for the analysis.


Figure 5.5: Left: Transmission for Sierpinski carpet of generation, $G=3$, with a width of: $W=27$ and Length: $L=27$. Right: Transmission for Sierpinski carpet of generation, $G=5$, with a width of: $W=243$ and Length: $L=243$. The amount of points computed is 2 times as small in both directions, compared to other results.

### 5.3.1 Bulk Modes

In the Hofstadter model we were able to identify the bulk modes via subtracting the transmission results of a smaller square from the of a larger square. The most natural way repeat this for the Sierpinski carpet is by subtracting the results of a smaller generation:

$$
\begin{equation*}
\Delta T=T(G=4)-T(G=3) \tag{5.2}
\end{equation*}
$$

The results of this are shown in figure 5.6. The result of this is substantially different from that of the Hofstadter model, as many regions contain increasing transmission close to regions of decreasing transmission. This is a result of more small scale details showing up in the transmission results. When investigating the localization of the states in the coloured regions of figure 5.6 , we obtain states that are localized through the entire lattice. As these states are also localized around the holes of the Sierpinski carpet, it makes sense that they are affected by an increase in fractal generation.


Figure 5.6: $\Delta T$ as defined in equation (5.2) combined with examples of state localization.

### 5.3.2 Chiral Edge Modes

In the square lattice model we were able to confirm the presence of edge modes by comparing observed plateaus of transmission to the theoretical predictions of the hall voltage $\sigma_{x y}$. Furthermore, we showed that these regions support states that indeed are localized on the edge. The transmission of these plateaus was not easily affected by impurities, because chiral modes are stable to impurities.

We do not have any predictions for the hall voltage for the Sierpinski fractal, but we can show that there are regions that have states localized on the edge and are stable to impurities. We investigate the resistance to impurities by adding a random impurity at each lattice point, $\mu_{i} \in[-0.3 t, 0.3 t]$. Then, in order to calculate the average transmission, $T_{A}$, and standard deviation, $\sigma$, we calculate the transmission 40 times with a different realization of the impurities. This is done for a mesh of flux and energy. The results of this calculation is shown in figure 5.7.


Figure 5.7: Up: Localization of edge states. The coloured dots show their locations in the energy flux plane in the other results. Down: The results for calculations with random impurities, $\mu_{i} \in[-0.3 t, 0.3 t]$, generated by 40 samples for a generation three Sierpinski carpet. Down-left: Average transmission, $T_{A}$. Down-right: Standard deviation, $\sigma$.

The results of figure 5.7 confirm that the regions with transmission one are stable to impurities and contain states that are localized on the edge. Thus, these regions support chiral edged modes. However not all areas that are resistant to noise have transmission one, there are many areas of transmission zero as well. So, in order to visualize were the single chiral edge modes are, we create a combined function

$$
\begin{equation*}
R=\left(T_{A}-1\right)^{2}+\sigma \tag{5.3}
\end{equation*}
$$

The results of $R \approx 0$ correspond to were the single chiral edge modes are. We show the results in figure 5.8.
We have confirmed the existence of single chiral edge modes, but one may wonder if there are regions containing multiple chiral edge modes. The regions of transmission two and four that we mentioned earlier as plateaus are not stable to impurities, so these do not contain chiral modes. Although no other large plateaus are observed, it is possible that a small region containing multiple chiral edge modes exists. To check if this is the case we look for a pixel that is stable to impurities and has a transmission larger than one. This was done by filtering out all pixels that have a high standard deviation, $\sigma>0.1$, and looking at the remaining pixels. A histogram of the pixels after filtering is shown in figure 5.8. No single pixel is found that has a transmission larger than one and a half. Thus we conclude no multiple edge modes exist.

One reason why no multiple edge modes exist, is that in the Hofstadter model the multiple edge modes have a localization that is multiple sites wide along the edge. The Sierpinski carpet creates holes such that the edge region is only a single site wide. This could disrupt the multiple edge modes.


Figure 5.8: Left: $R$ as defined in equation (5.3) for Sierpinski carpet of generation three. Right: The frequency of pixels ranked by their value for the transmission, $T$, after filtering out all pixels with $\sigma>0.1$.

### 5.3.3 Non-Chiral Edge Modes

In figure 5.4 we observe a plateau region in the centre with a transmission of approximately 2 . We also mentioned there was a region of transmission 4. The presence of these regions and the fact that they remain constant over multiple generations is best shown through the scaling function

$$
\begin{equation*}
S=\frac{T(G=4)}{T(G=3)} \tag{5.4}
\end{equation*}
$$

Here, $S$ is set to zero if the transmission of either $G=3$ or $G=4$ is smaller than $1 / 10$. The results of $S\left(E / t, \Phi / \Phi_{0}\right)$ are shown in figure 5.9. We are interested in the regions where $S \approx 1$, which implies that the transmission is the same in both generations. We see that the regions with chiral edge modes are contained in figure 5.9, this means that the chiral modes are present across different generations. Yet there are two regions that do not contain chiral edge modes. The first such region is near $\left(E / t=0, \Phi / \Phi_{0}=0\right)$. This region contains states that form a cross and diamond shape as was shown in figure 5.3.


Figure 5.9: Up: Examples of the localization. Down-left: $S\left(E / t, \Phi / \Phi_{0}\right)$ as defined in equation (5.4). Downright: transmission for a slice at $\Phi / \Phi_{0}=0.48$.

The second region constant under scaling is near $\left(E / t=0, \Phi / \Phi_{0}=1 / 2\right)$. Slicing through the flux plane at $\Phi / \Phi_{0}=0.48$ reveals a sinusoidal pattern. The localisation of the states in the sinusoidal region consists entirely of states that are localized on the edges. The cause of this behaviour might be related to the shape of the edge states. We see that the edge states loop around the smallest holes that have been cut out to create the Sierpinski fractal. This creates states that schematically look like figure 5.10.


Figure 5.10: Sketch of the localization of states in the $T=2$ plateau.
This region is not stable to impurities and there are two channels for transport. This suggests that there are two modes, but they have opposite chirality. These two modes can then scatter from a left moving mode to a right moving mode at an impurity, thus explaining why these modes are not resistant to impurities. We think that the localization of these states, as we illustrate in figure 5.10, has a relation to this behaviour.

### 5.3.4 Conclusion

By comparing the transmission results for different generations, we find that the transmission is mostly identical across generations. A major exception to this is what might be called the 'bulk region', were each successive generation adds more small scale structure. The states in this region are found to be localized
through the entire lattice, this combined with literature $[6,5]$ suggests that this increase in small scale structure is related to the fractal nature of the lattice.

The regions that persists across different generations may be divided into three categories: The first and most important category is the chiral edge mode area. These regions are stable to impurities, have transmission one and contain states localized on the edge. No regions are found that are stable against impurities and with transmission more than one. So we rule out multiple chiral modes, unless their domains are smaller than the mesh used.

The remaining two regions are not stable against impurities and have a transmission of two and four. The plateau with transmission two also contains states localized on the edge and are non-chiral. A hypothesis as to why this state has no chirality was put forward, in the discussion the steps to check this will be disused. The plateau with transmission four contains modes resembling cross and diamond structures and are non-chiral.

## Chapter 6

## Discussion

In this thesis we verified the existence of chiral edge modes by observing that there are regions of transmission one, that are resistant to noise. But we can not distinguish between chiral edge modes with a positive Hall conductivity, $\sigma_{x y}$, and negative Hall conductivity. We know that in the Hofstadter model there are regions of positive Hall conductivity and negative Hall conductivity, so a similar behaviour is expected for the Sierpinski carpet results.

To measure the hall conductivity, a set-up with leads at the edges is required, this set-up is shown in figure 6.1. Such a set-up may be described by an extension of the procedure described in chapter 3. For this extension the Landauer-Büttiker formalism has transmission functions between each lead: $T_{1 \rightarrow 2}, T_{1 \rightarrow 3}$, $T_{2 \rightarrow 3}$, etc. These transmission function may each be calculated by the same recursive procedure, but some modification is required to include the new leads. This implementation is beyond the scope of this thesis, but this was done by associated research [36]. The results of this associated research are also shown in figure 6.1. These results align with the conclusions from this thesis, as only single edge modes and in the same regions are found.


Figure 6.1: Left: Set-up of a system that can measure the Hall conductivity, $\sigma_{x y}$. Right: Results for the Hall resistivity for the set-up shown on the right, for a generation 4 fractal. These results are from [36].

For the Non-chiral edge modes discussed in section 5.3 .3 we gave a hypothesis of the mechanism that causes them. To check this hypothesis, further investigation of the wave functions may provide answers. The wave
functions where found by directly diagonalising the Hamiltonian, but we only used the absolute value squared to show how these states are localized. By investigating the differences in phase between neighbouring lattice sites, the local momentum may be found. This may be used to find the chirality of the mode. Furthermore if one where to sum the difference in phase along a closed path, the total phase should add up to $2 \pi n$ with $n$ an integer. Then we could calculate this number for the path along the boundary, but also for the holes of the Sierpinski carpet. The expectation is that using this one would be able to independently confirm the chirality of the modes. This might enable one to also decompose the non-chiral modes into the two different chiralities.

The last point of interest is to further classify the states found by direct diagonalization. Currently this data was used to take a peek into how states in a certain energy region are localized. But by categorizing the states using an algorithm more information might be obtained. First of it should be straightforward to separate bulk states from edge states by filtering results based on their localization on the edge. This would provide a easy way of confirming that the chiral edge mode regions only contain states localized on the edges. It might also be possible to separate the bulk states into different family's. One way of doing this could be by comparing the localizations on different holes in the Sierpinski carpet. If one where to successfully classify the states one could compare these family's for different generations of the Sierpinski carpet and investigate the scaling and self-similarity of the states across the generations.

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