Energy filtered leads for quantized transport in Floquet systems

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Abstract

Topological insulators are exotic phases of matter that display a variety of interesting physical phenomena. Unlike other insulators these systems are characterized by perfectly conducting states at the edge, that are robust and universal in nature. Recently it was proposed that non-equilibrium phases dubbed Floquet topological insulators could be created using time periodic external fields. Unlike their equilibrium counterpart these new exotic states of matter do not generally display the same physical features. Signatures such as conductance quantization which is present in equilibrium topological phases are absent in Floquet topological insulators due to photon-assisted tunneling. Recently it was proposed that quantization could be restored in these systems by using so called energy filtered leads. In this thesis, we study this strategy from a theoretical viewpoint. Using non-equilibrium Green’s functions, numerical results for various physical quantities of these systems are obtained. We find that our method leads to almost perfectly quantized values of differential conductance. In addition several other physical quantities are obtained that further support our results. The method used here can be applied the several other periodically driven topological systems where photon assisted tunneling spoils conductance quantization.
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Chapter 1

Introduction

Topological phases of matter is arguably one of the most intriguing topics in modern condensed matter physics. It all started when von Klitzing and co-workers discovered the quantum Hall effect in 1980 [1]. Specifically von Klitzing and co-workers showed that at low temperatures a two dimensional electron gas (2DEG) in an external magnetic field exhibits robust plateaus in the Hall resistivity regardless of the choice of material, disorder and external perturbations. It soon became clear that the robustness of the quantum Hall plateaus could be stood in terms of topology [2]. Since then topology has gone from an explanation of the quantum Hall effect to a guiding principle in condensed matter physics. Since the early 1980’s theorists have predicted many new interesting phases of matter simply by looking for a topological structure in the models of these systems. In particular so called topological insulators were discovered not long after their theoretical prediction [3, 4]. These new materials are the hosts of special quantum states that are protected by topology and consequently have many physically interesting phenomena associated with them [5]. Classifying these phases and discovering what new physical phenomena they give rise to have been a major focus in condensed matter physics over the last 20 years. A specific class of these topological insulators was predicted to exhibit quantized Hall response just like in the two dimensional electron gas, but without an external magnetic field [6]. The explanation was that the underlying topological structure is similar to the system discovered by von Klitzing. Despite this theoretical triumph many of the phenomena predicted by theorists have not yet been seen in experiments. The theoretically predicted models are either not realistic or can only be observed in a very limited number of materials. Recently periodic driving was suggested as a possible tool to create topological materials [7, 8]. Subsequently it has been shown theoretically that periodic driving could be used to create several of the topological phases known in non-driven systems [7, 10, 11]. There has even been recent work which predicts new topological phases with no counterpart in equilibrium systems [12]. Recently it was proposed that the so called Chern insulator, originally predicted in 1988 [6], could be created by shining circularly polarized light on a graphene sample [7]. It has been predicted that this system exhibits quantized Hall conductivity [7, 9], just like its equilibrium counterpart [6]. The problem is that this driven system is no longer an equilibrium system. Therefore it is not trivial how electrons will populate such a system. In order to observe quantized transport the steady state distributions of periodically driven systems have to resemble that of an equilibrium topological insulator [7]. Recently it was suggested that it is possible to control the steady state of periodically driven systems by coupling these systems to carefully tailored external baths [13]. In particular it was shown that leads with a narrow bandwidth, so called energy filtered leads, could be used to engineer a more ideal steady state in periodically driven topological insulators. In real transport experiments such energy filters could be used to not only control the steady state but also to suppress photon assisted tunneling processes [14]. These processes are a general feature of periodically driven systems and for a topological insulator they spoil the conditions that usually lead to quantized conductance, which is one of the hallmarks of non-driven topological insulators. The study of transport in driven systems with energy filtered leads has already been the subject of study in some recent work [15]. While the results are promising, a direct computation of the conductance from first principles has not yet been done \(^{1}\). In this thesis the first study of transport through a driven system with energy filtered leads is presented. The conductance through a two terminal setup is directly computed using a numerical non-equilibrium Green’s function approach. These results are compared to those obtained from a more conventional transport setup with a driven topological insulator that has wide band leads attached. In addition to computing the conductance the

\(^{1}\)To the best of my knowledge.
non-equilibrium Green’s function technique is further utilized to find the spatial distribution of particles and current as well as non-equilibrium distribution functions which give further insight into the effect of energy filtered leads.

1.1 Thesis outline

The first chapters of the thesis are meant to give a brief but coherent overview of periodically driven systems, topological insulators and quantum transport. Since these are all a whole research area of their own the emphasis of each chapter is on the topics and concepts relevant to understanding the goal of this thesis. The focus of each chapter is to discuss physical ideas and concepts. Therefore most of the long or technical computations that lead to the results stated in the main text are given in appendices. Hopefully this will make for a more coherent reading experience where each step is clear and motivated.

The chapters in the thesis are organized as follows

- In chapter 2 the basics of the Floquet theory framework is introduced. The Floquet theorem is introduced, it is explained how this can help analyze periodically driven systems. The extended space formalism is introduced and it is explained how this can be used to map a time periodic problem to a time-independent one. These concepts will form the backbone of the analysis done in the subsequent chapters of the thesis.

- Chapter 3 introduces topological insulators. First a general discussion of non-driven topological insulators is given. The most central concepts such as topological invariants and bulk-edge correspondence are covered. Subsequently Chern insulators are introduced. A concrete example of such an insulator is given to illustrate some of the properties of this particular topological insulator. Finally Floquet topological insulators are introduced. It is explained how periodic driving may generate Hamiltonians with a topologically non-trivial structure. Furthermore some of the essential differences between Chern insulators and Floquet topological insulators are discussed.

- Chapter 4 concerns quantum transport through periodically driven systems and what physical quantities may be observed in such settings. The Keldysh formalism is introduced and subsequently it is shown how non-equilibrium Green’s functions can be used to obtain desired physical quantities such as time-averaged differential conductance, time-averaged particle- and current density as well as non-equilibrium distribution functions.

- In chapter 5 the recursive Green’s function technique is introduced to help obtain the Green’s functions introduced in the previous chapter. First the necessity of this algorithm is explained. The idea behind the algorithm is then presented as well as a more technical discussion of how the algorithm works. Finally it is shown how this algorithm should be used for periodically driven systems.

- Chapter 6 culminates with a presentation of results, obtained using the formalism developed in the first five chapters. This is where new results are presented and discussed. First the model introduced in the end of Chapter 3 is used to demonstrate some of the issues with transport trough driven systems coupled to wide band leads. Numerical results for the time-averaged differential conductance using the formalism introduced in Chapters 4 and 5 are presented and discussed. Subsequently a model for an energy filtered lead is introduced and used to define a modified two terminal setup. The time-averaged differential conductance for this system is also found and is then compared to the one obtained for the same system without energy filtered leads. In addition results for particle and current densities of the new setup are found to be in good agreement with the result for the time-averaged conductance. Furthermore non-equilibrium distribution functions for both setups are found and compared. Finally a discussion of possible implementation of this strategy in experiments is given.

- Finally chapter 7 concludes with a discussion of the results presented in this thesis, as well as a discussion of future work within the field.
Chapter 2

Floquet theory

Periodically driven systems is a rich class of systems with many interesting features that makes them special compared to other dynamical systems. The reason why so much can be said about these systems is that there exists a natural framework in which these systems can be described, called Floquet theory, which is briefly introduced in this chapter. There are many excellent papers and reviews on the topic, this chapter however is based on what is written in [14] and [16]. Throughout this chapter we set $\hbar = 1$.

2.1 Periodically driven quantum systems and the Floquet theorem

It is well known that the dynamics of a quantum system is described by the Schrödinger equation:
\[ i \frac{d}{dt} \ket{\Psi(t)} = H(t) \ket{\Psi(t)}, \]  
where $H(t)$ is the Hamiltonian of the system of interest and $\ket{\Psi(t)}$ is the state of the system. Quantum dynamics is generally difficult to analyze, since there are only few known exact solutions to the time-dependent Schrödinger equation. However there exists a certain class of systems where the solutions to Eq. (2.1.1) take on a particular form. In particular quantum systems that are described by Hamiltonian’s that are periodic in time can be studied using the framework of Floquet theory. Floquet theory is the study of differential equations of the form:
\[ \frac{d}{dt} x(s,t) = A(s,t) x(s,t), \]  
where $A(s,t)$ is a linear operator with the property $A(s,t) = A(s,t+T)$. $x(s,t)$ is a vector, $s$ is a set of parameters and $t$ denotes the time variable. Floquet theory has applications in many different areas of physics, however here the focus is to apply the framework to periodically driven quantum systems. Suppose that we are studying a quantum system that is governed by a Hamiltonian which is periodic in time. That is the Hamiltonian satisfies $H(t+T) = H(t)$, where $T$ denotes the period of the Hamiltonian. In this case the time-dependent Schrödinger equation has the same form as Eq. (2.1.1). Typically such a time-periodic Hamiltonian can be realized by adding an external periodic field such as a periodic magnetic field or a laser pulse. The essence of Floquet theory is the so called Floquet theorem. The Floquet theorem states that the solutions $\ket{\Psi_\alpha(t)}$ to the time-dependent Schrödinger equation can be written as [17]:
\[ \ket{\Psi_\alpha(t)} = e^{-i\epsilon_\alpha t} \ket{\Phi_\alpha(t)}, \]  
where the parameter $\epsilon_\alpha$ is a known as the quasienergy and the states $\ket{\Phi_\alpha(t)}$ are known as Floquet states. Furthermore these states satisfy $\ket{\Phi_\alpha(t)} = \ket{\Phi_\alpha(t+T)}$. To analyze the problem further it is useful to define the operator
\[ H_F(t) = H(t) - i \frac{d}{dt}. \]  
This is known is the Floquet Hamiltonian\(^1\). The Floquet Hamiltonian has several important properties. First of all the Floquet Hamiltonian is to periodically driven systems what the Hamiltonian is to a

\(^1\)Confusion sometimes arises in the literature since the term Floquet Hamiltonian may sometimes also refer to the effective Hamiltonian which governs the dynamics of a periodically driven system over one period [18].
time-independent system. To see this we apply the Floquet Hamiltonian to a Floquet state. Using Eqs. (2.1.3) and (2.1.4) one finds that:

\[ H_F(t) \left| \Phi_\alpha(t) \right\rangle = (H(t) - i \frac{d}{dt})(e^{i\epsilon_\alpha t} \left| \Psi_\alpha(t) \right\rangle) \]

\[ = e^{i\epsilon_\alpha t} \left( (H(t) \left| \Psi_\alpha(t) \right\rangle - i \frac{d}{dt} \left| \Psi_\alpha(t) \right\rangle) + \epsilon_\alpha \left| \Psi_\alpha(t) \right\rangle \right) \]

\[ = e^{i\epsilon_\alpha t} \epsilon_\alpha \left| \Psi_\alpha(t) \right\rangle = \epsilon_\alpha \left| \Phi_\alpha(t) \right\rangle. \] (2.1.5)

This calculation shows that the Floquet states are eigenstates of the Floquet Hamiltonian. Furthermore the Floquet Hamiltonian is Hermitian. Therefore it follows that the quasienergies must always be real numbers. If we think about the quasienergy as the generalization of normal energy for periodically driven systems Eq. (2.1.5) bears a close resemblance to the time-independent Schrödinger equation. In fact we can expand any state \( |\Psi(t)\rangle \) of a periodically driven system in terms of Floquet states:

\[ |\Psi(t)\rangle = \sum_\alpha c_\alpha e^{-i\epsilon_\alpha t} |\Phi_\alpha(t)\rangle, \] (2.1.6)

where \( c_\alpha = \langle \Phi_\alpha(0)|\Psi(0)\rangle \). The expansion in Eq. (2.1.6) looks just like the expansion of a quantum state in terms of stationary states for the time-independent problem. However the Floquet states are of course time-dependent. We now make the observation that we can construct new solutions to Eq. (2.1.1) by defining new Floquet states

\[ |\Phi_\alpha'(t)\rangle = e^{i\Omega t} |\Phi_\alpha(t)\rangle, \] (2.1.7)

where \( n \) is an integer and \( \Omega \) is the driving frequency given by \( \Omega = \frac{2\pi}{T} \). These new Floquet states are also periodic in time. Furthermore they are also eigenstates of the Floquet Hamiltonian. To see this we use Eq. (2.1.5) to get

\[ H_F(t) \left| \Phi_\alpha'(t) \right\rangle = (H(t) - i \frac{d}{dt})e^{i\Omega t} |\Phi_\alpha(t)\rangle \]

\[ = e^{i\Omega t}( (H(t) - i \frac{d}{dt}) + n\Omega) |\Phi_\alpha(t)\rangle \]

\[ = e^{i\Omega t}(\epsilon_\alpha + n\Omega) |\Phi_\alpha(t)\rangle = (\epsilon_\alpha + n\Omega) |\Phi_\alpha'(t)\rangle. \] (2.1.8)

It is clear that the new Floquet states are also eigenstates of the Floquet Hamiltonian but with their quasienergies shifted by integer multiplies of \( \Omega \). For each Floquet state \( |\Phi_\alpha(t)\rangle \) it is always possible to construct new states \( |\Phi_{\alpha n}\rangle \) using Eq. (2.1.7). These Floquet states are physically identical to the old ones since they correspond to the same solution to the time-dependent Schrödinger equation \( |\Psi(t)\rangle \). To distinguish the solutions that are unique from the ones that are not, it is useful to define the first Floquet zone, in analogy with the first Brillouin zone for spatially periodic systems [20]. That is a finite zone where the quasienergy satisfy

\[ -\frac{\Omega}{2} < \epsilon_\alpha < \frac{\Omega}{2}. \] (2.1.9)

For any \( \epsilon_\alpha \) in the Brillouin zone there are infinitely many quasienergies \( \epsilon_\alpha + n\Omega \) outside the zone which correspond to physically identical solutions to the Schrödinger equation. The quasienergy allows us to give meaning to the notion of spectra in a similar way to what is done for time-independent Hamiltonians. The catch is that the quasienergies are periodic which means that quasienergy is a quantity that exists on a circle. This has many striking consequences. For instance it is impossible to unambiguously define a ground state for a periodically driven system. To be instructive it is nice to give an example of how the quasienergy concept works in the context of condensed matter physics. The attentive reader will have noticed a similarity between the Floquet theorem presented here and the well known Bloch theorem from textbook band theory [20]. In fact the periodicity of the quasienergy and the form of the solutions closely resembles Blochs theorem for non-driven systems. In fact the Bloch theorem is mathematically identical to the Floquet theorem. In the same way that Bloch bands are formed in a crystal with discrete spatial symmetry periodically driven systems forms so called Floquet bands. If the periodically driven system also has discrete spatial symmetry the bands are called Floquet-Bloch bands. An example of both types of bands can be seen in Fig. 2.1.

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2 The Floquet theorem dates back to 1883. Bloch re-discovered this theorem in 1928.
2.2 Extended space formalism

Due to their time-periodicity each Floquet state has a Fourier decomposition

$$ |\Phi_\alpha(t)\rangle = \sum_{n=-\infty}^{\infty} |\phi_n^{(\alpha)}\rangle e^{in\Omega t} $$  (2.2.1)

We already saw that there was a redundancy to the definition of Floquet states in the sense that

$$ |\Phi_{\alpha,p}(t)\rangle = e^{ip\Omega t} |\Phi_\alpha(t)\rangle $$  (2.2.2)

is also a Floquet state. Therefore for each Floquet eigenstate one can form a class $\alpha' = (\alpha, p)$. This physically identical state has the decomposition

$$ |\Phi_{\alpha,p}(t)\rangle = \sum_{n=-\infty}^{\infty} |\phi_n^{(\alpha,p)}\rangle e^{in\Omega t} = \sum_{m=-\infty}^{\infty} |\phi_n^{(m-p)}\rangle e^{im\Omega t}, $$  (2.2.3)

where $m = n + p$. Therefore there is a certain symmetry between the components: $|\phi_n^{(m-p)}\rangle = |\phi_n^{(m)}\rangle$. In the literature these components are called sidebands. In time-independent quantum mechanics we usually work with stationary states. These states form a complete set, meaning that any state in can be expressed in terms of them and that they satisfy an orthonormality relation:

$$ \sum_n |n\rangle \langle n| = \mathbb{1}, \quad \langle n|n'\rangle = \delta_{nn'} $$  (2.2.4)

The Floquet states are not entirely stationary states, their time-dependence however is periodic. A Hilbert space of period functions has the inner product:

$$ (u, v) = \frac{1}{T} \int_0^T u^*(t)v(t) dt $$  (2.2.5)

Any function in such a Hilbert space can be expanded in terms of the functions $\exp(im\Omega t)$ with $m = 0, \pm 1, \pm 2...$ that form a complete set in this space. Therefore when working with Floquet states it is useful to separate the Hilbert space into two parts. It is custom to introduce the composite space $F = \mathbb{R} \otimes T$. Due to the separation in the decomposition in Eq. (2.2.3) all the time dependence is packed into the functions $\exp(im\Omega t)$ and they span the space $T$. The physical space $\mathbb{R}$ is spanned by the states $|\phi_n^{\alpha}\rangle$. The space $F$ is known as the extended space and it is spanned by the states $|\Phi_\alpha\rangle$ [21]. We may then similarly define an inner product for this composite space as:

$$ \langle\langle \Phi_{\alpha,p}|\Phi_{\beta,q}\rangle\rangle = \frac{1}{T} \int_0^T \langle\Phi_{\alpha,p}(t)|\Phi_{\beta,q}(t)\rangle dt = \delta_{\alpha\beta}\delta_{p,q}. $$  (2.2.6)
A crucial detail is that two Floquet states are only orthogonal at equal times. At equal times the Floquet states of the first Floquet zone already form an orthonormal set in $\mathbb{R}$:

$$\sum_\alpha |\phi_{\alpha,0}(t)\rangle \langle \phi_{\alpha,0}(t)| = \mathbb{I}. \quad (2.2.7)$$

If the two times are different however this is no longer enough. The decomposition in extended space can be used to reformulate Eq. (2.1.5) as a time-independent equation. Because all times are equal we only need to consider states belonging to the same class. We therefore focus on the class where $p = 0$. Because we are also considering time-periodic Hamiltonians they also have a Fourier decomposition

$$H(t) = \sum_{k=-\infty}^{\infty} H_k e^{-ik\Omega t} \quad (2.2.8)$$

In the extended space the matrix elements $H_{nm}$ then become:

$$H_{mn} = \frac{1}{T} \int_0^T dt e^{-im\Omega t} H(t)e^{im\Omega t} = H_{m-n}. \quad (2.2.9)$$

We can now recast the eigenvalue equation by writing:

$$\left( H(t) - i \frac{d}{dt} \right) \sum_{n=-\infty}^{\infty} e^{i\Omega n t} |\phi^{(n)}_\alpha\rangle = \epsilon_\alpha \sum_{n=-\infty}^{\infty} e^{i\Omega n t} |\phi^{(n)}_\alpha\rangle \quad (2.2.10)$$

We now multiply on both sides by $e^{(-im\Omega t)}$ and take the time average on both sides of Eq. (2.2.10) to get:

$$\sum_{n=-\infty}^{\infty} \frac{1}{T} \int_0^T dt \left( e^{-im\Omega t} H(t)e^{im\Omega t} - ie^{-im\Omega t} \frac{d}{dt} e^{im\Omega t} \right) |\phi^{(n)}_\alpha\rangle = \epsilon_\alpha \sum_{n=-\infty}^{\infty} e^{i(m-n)\Omega t} |\phi^{(n)}_\alpha\rangle$$

$$\iff \sum_{n=-\infty}^{\infty} (H_{m-n} + \delta_{mn} \Omega) |\phi^{(n)}_\alpha\rangle = \epsilon_\alpha |\phi^{(m)}_\alpha\rangle. \quad (2.2.11)$$

We see that Eq. (2.2.11) constitutes a set of coupled equations. Furthermore this set of equations are completely independent of time. In the extended space this may in fact be seen as an eigenvalue equation if we use the following matrix structure:

$$\begin{pmatrix}
\ddots & \ddots & \ddots & \ddots \\
\ddots & H_0 + \Omega & H_1 & H_2 \\
\ddots & H_{-1} & H_0 & \ddots \\
\ddots & H_{-1} & H_{-2} & \ddots \\
\ddots & \ddots & \ddots & \ddots \\
\end{pmatrix}
\begin{pmatrix}
|\phi^{(1)}_\alpha\rangle \\
|\phi^{(0)}_\alpha\rangle \\
|\phi^{(-1)}_\alpha\rangle \\
\ddots \\
|\phi^{(1)}_\alpha\rangle \\
\end{pmatrix}
= \epsilon_\alpha
\begin{pmatrix}
|\phi^{(1)}_\alpha\rangle \\
|\phi^{(0)}_\alpha\rangle \\
|\phi^{(-1)}_\alpha\rangle \\
\ddots \\
|\phi^{(1)}_\alpha\rangle \\
\end{pmatrix} \quad (2.2.12)$$

This eigenvalue equation exists in the extended Hilbert space where each component $H_{m-n}$ has the dimension of the original Hilbert space. The blocks on the diagonal represent copies of the Fourier component $H_0$, but shifted in quasienergy by multiples of $\Omega$. The effect of the external drive is to couple the different blocks $H_0 - n\Omega$ together. In principle all the different sidebands $|\phi_{\alpha,n}\rangle$ are need to obtain the Floquet state $|\phi_\alpha(t)\rangle$. For sufficiently weak driving amplitude and sufficiently high driving frequency it is often enough to keep only a finite number of the Floquet sidebands. This allows one to truncate the extended space into a finite $(2M + 1) \otimes \text{dim}(\mathbb{R})$ dimensional space and then use the resulting finite matrix to find Floquet modes as well as the quasienergy spectrum. Typically this has to be done numerically. The advantage is that one can always compute results for a given truncation and then perform the same computation with additional copies. Repeating this procedure until the result converges is a practical way to ensure enough copies are kept. Now that the basic theory of periodically driven systems have been covered we can turn our attention to the particular systems of interest for this thesis, namely topological insulators.
Chapter 3

Topological Insulators

This chapter introduces topological insulators for non-driven as well as driven systems. First the general features of non-driven topological insulators are explained. We then turn our attention to a particular family of topological insulators, the so called Chern insulators. Subsequently we study the features of Chern insulators within a concrete toy model, first introduced by Haldane. We then discuss periodic driving as an alternate route to generate a non-equilibrium analog of Chern insulators, so called Floquet topological insulators. To do so we introduce a recently proposed model, where circularly polarized light is used to tune the topological properties of the two dimensional system graphene. We study this model in different frequency regimes and discuss different mechanisms for generating gaps in the spectrum of the system. Finally we discuss some of the main differences between Floquet topological insulators and their static counterparts and the issues that arise due to these differences.

3.1 General features topological insulators

We begin this section by introducing non-driven topological insulators [5]. Specifically we will consider non-interacting, time-independent systems of fermions. To study the bulk properties of these systems we also require that the systems have discrete translational invariance. These systems are described by a time-independent Hamiltonian $H$. In addition to the requirements already stated we also require that this Hamiltonian is local. That is the Hamiltonian can only contain terms that couples points in space that are adjacent to each other. Due to translational invariance crystal momentum will be a good quantum number and the eigenstates and eigenenergies can be found from the time-independent Schrödinger equation:

$$H |\Psi_k\rangle = E(k) |\Psi_k\rangle. \quad \text{(3.1.1)}$$

According to Bloch’s theorem the eigenstates of the Hamiltonian for such a system are Bloch states. That is a state which is a plane wave modulated by some spatially periodic function [20]. We know from band theory that the spectrum will consist of bands with forbidden regions in between them. If the Fermi energy lies inside the forbidden region between two bands the system is an insulator. Due to the locality condition this description is good even in a finite system as long as the system is sufficiently large and that only the bulk of the system is considered. If we consider a finite system, the description above breaks down near the edge. At the edge the potential is no longer periodic. Instead it starts to increase in size. This leads to distortion of the single particle wavefunctions which in some cases can lead to localized edge states. The energy of these edge states bends up in energy for an increasing potential at the edge which means their eigenenergies will lie in the forbidden gap. For a normal insulator the absence or presence of edges states as described here depends on the details of the system boundary. For instance the two dimensional material graphene has two different edge types: zig-zag and armchair edges. The zig-zag configuration supports edge states, but the armchair configuration does not. There is however a different class of insulators where edge states also appear, but are not characterized by the details of the system boundary. Here the edge states are instead characterized by details of the bulk despite the fact that the states themselves are localized at the edge. These materials are known as topological insulators. What distinguishes the bulk of these insulators from the bulk of a topologically trivial insulator is that they carry a so called topological invariant. A topological invariant is a number that cannot change continuously but only discretely. This number is carried by the bulk in the sense that it is obtained from the wavefunctions which are found from a bulk Hamiltonian $H$ as described
above. It is the underlying Hilbert space of this Hamiltonian that determines the topological structure
1. The existence of a topological invariant in the bulk manifests itself physically in the following way.
For topological insulators a topological invariant can be associated with each band in the insulator. This
invariant doesn’t change under smooth deformation of the bands as long as the deformation doesn’t cause
one or more bands to touch and close the bandgap between them. Therefore it is possible to assign an
equivalence class of topological insulators for which the topological invariant of each band is the same.
We now consider two insulators with the same dimensionality and equivalent symmetries. Furthermore
let us assume that they are topologically equivalent, that is the topological invariant of all their bands
assumes the same value. Then it is possible to deform the bands of one of the insulators into the bands
of the other insulator smoothly without closing the bandgap somewhere in the spectrum of the deformed
insulator. If two states are topologically distinct however, a gap must close and reopen somewhere in the
spectrum in order to deform the bands of one insulator such that they are the same as the bands of the
other insulator and vice versa. Topological invariants are very robust against small perturbations of the
bulk system such as weak disorder or weak interactions. Such effects will only distort the bandstructure a
little and as long as the gap stays open they do not change the topological invariant. Intriguingly it turns
out that the existence of edge states in topological insulators is due to the existence of some topological
invariant of the bulk. This is known as the bulk edge correspondence. Because the topological invariants
are robust so are the edge modes. Like the edge states of trivial insulators, topological edge states have
eigenenergies inside the bandgap. In Fig. 3.1 a topological insulator with its spectrum projected onto
one of its momenta is depicted. This particular model has two bands and an edge mode in the gap. The
mode is gapless in the sense that the edge mode closes the gap in the spectrum and connects the two bulk
bands, in contrast to the spectrum of the bulk alone, which is gapped. A mode should be understood
as all the states on the line connecting two bands, while the term edge state refers to one particular
state with crystal momentum k. The only way to remove an edge mode is to bring together two bands
thereby closing the bandgap. In fact the existence of edge modes in topological insulators can be seen as a
necessity from the following argument [22]. Let us consider a topological insulator that is in proximity to
a trivial insulator, that is an insulator without gapless states. If we study the spectrum of this two piece
system as a function of distance the gap has to close somewhere otherwise the spectrum of one insulator
can be deformed into the spectrum of the other insulator without closing a gap in the insulator. This is
a contradiction however since then the two insulators wouldn’t be topologically distinct. Therefore the
spectrum has to be gapless somewhere. The edge states of the topological insulator reside on its edge.
This edge is also the interface between the two insulators and it is here that the system becomes gapless.
The states deep in the bulk of both materials lie in the bulk bands and do not change. However at the
edge the topological insulator has states with energies in the gap that causes the system to be gapless
in this region as required for the topological invariant to change.

![Figure 3.1: Bandstructure of topological insulator.](image)

The discussion so far has been general but there are many additional features or physical phenomena

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1More precisely it is a certain set of maps from the parameter space, which consist of the crystal momenta k, onto the
Hilbert space \( \mathcal{H} \) that are topological. A set of maps with the same topology form what mathematicians call a homotopy
class.
which are tied to specific types of topological insulators. In order to tell these different insulators apart, physicists have classified topological insulators by their symmetry class. Depending on what discrete symmetries are present and what dimensionality is considered different topological insulators with different topological invariants may arise. A complete classification has been given for non-interacting, non-driven systems [23, 24]. For non-interacting periodically driven systems a topological classification has also been carried out. However due to the periodicity of quasienergy periodically driven topological insulators have a more rich topological structure. We will discuss this briefly later in this chapter.

3.2 Haldane’s Chern insulator

To demonstrate the concepts of the previous section we will now discuss a particular class of topological insulators, the so called Chern insulators. We will consider a specific toy model, namely Haldane’s Chern insulator which is historically the first example of a Chern insulator. The model was introduced by Haldane in 1988 [6]. The Haldane model describes spinless fermions on a 2D honeycomb structure. The unit cell for this lattice has two atoms. This means that the system has two bands which is the minimal requirement to obtain a topological insulator. The sites on the lattice are connected by the nearest neighbor vectors

\[ \delta_1 = \frac{a}{2}(1, \sqrt{3})^T, \quad \delta_2 = \frac{a}{2}(1, -\sqrt{3})^T, \quad \delta_3 = a(0, -1)^T. \]

The lattice is spanned by the reciprocal lattice vectors:

\[ a_1 = \frac{a}{2}(3, \sqrt{3})^T, \quad a_2 = \frac{a}{2}(3, -\sqrt{3})^T. \]

We also define an additional vector:

\[ a_3 = a_1 - a_2 = a(0, \sqrt{3})^T. \]

The vectors \( a_1, -a_1, a_2, -a_2, a_3 \) and \(-a_3\) are the vectors connecting a site to its next nearest neighbors. The Haldane model is a lattice tight-binding model with three terms

\[ H_{\text{Haldane}} = H_{NN} + H_M + H_{NNN}. \]

The first part is a tight-binding term with nearest neighbor hopping only:

\[ H_{NN} = J_1 \sum_{\langle ij \rangle} \left( c_i^\dagger c_j + \text{h.c.} \right). \]

Here \( J_1 \) denotes the nearest neighbor hopping parameter and \( c_i^\dagger \) and \( c_j \) denote fermionic creation and annihilation operators for site \( i \) and site \( j \) respectively. This first term is often used to describe the two dimensional material graphene. This material consists of carbon atoms alone and the nearest neighbor hopping term gives rise to the \( \pi \)-bands in graphene [25]. The second term in the Haldane model is an inversion breaking term

\[ H_M = M \sum_i \left( c_{i,A}^\dagger c_{i,A} - c_{i,B}^\dagger c_{i,B} \right), \]

where the sum is over the number of sites on one sublattice. This term simply adds an on site potential \( M \) with opposite sign on sublattice \( A \) and sublattice \( B \). The final term in the Haldane Hamiltonian is a second nearest neighbor hopping term:

\[ H_{\text{NNN}} = J_2 \sum_{\langle (il) \rangle \sigma} \left( e^{-i\phi_{l,\sigma}^i} c_{i,\sigma}^\dagger c_{l,\sigma} + \text{h.c.} \right), \]

where the sum \( i \) is over the number of sites on one sublattice and the parenthesis \( \langle \cdot \rangle \) means that the \( l \) sum only includes second nearest neighbors. The complex hopping parameter is given by \( J_2 e^{i\phi} \) and the complex phases on these hopping parameters are chosen such that for a given sublattice the sign of the complex phases alters between bonds of different next nearest neighbors. For instance for sublattice \( A \) the hopping parameter between a site and its next nearest neighbors \( 1, 3, 5 \) gets a complex phase \( \exp(i\phi) \) and similarly the hopping parameter from the same site to its next nearest neighbors \( 2, 4, 6 \) gets a phase
of exp(−iφ). The same principle applies to sublattice B however with the opposite sign convention. The complex phases on the next nearest neighbor term arise from a magnetic field that varies periodically in space with the same period as the hexagonal lattice. This leads to a magnetic flux

\[ \phi = \frac{e}{\hbar} \oint A(r) \cdot dr = \frac{e}{\hbar} \oint_{\mathcal{S}} B(r) \cdot d\mathcal{S}, \]

(3.2.8)

where \( A(r) \) is the electromagnetic vector potential, \( B(r) \) is the resulting magnetic field and \( \phi \) the magnetic flux. The line integral is over a closed loop which encircles a plaquette if the path taken involves only nearest neighbors. The area encircled is a triangle if next nearest neighbors are used. Because the magnetic field is constructed this way the overall magnetic flux through each plaquette in the lattice is zero. Therefore the nearest neighbor term does not have any complex phase. The actual magnetic field is still non-zero and time reversal symmetry is therefore broken. Complex phases such as the ones in Eq. (3.2.7) arise naturally when a magnetic field is added to a tight-binding model. This is known as Peierls substitution and it is a way to add the magnetic field to a lattice model. It is equivalent to the minimal coupling procedure where the momentum of a particle is modified as \( k \rightarrow k - eA \). In order to ensure that the Hamiltonian in Eq. (3.2.4) describes an insulator we furthermore require that \( \frac{k_j^2}{N} < \frac{1}{4} \) [6]. Although there is a reasonable physical motivation behind the Haldane model, it has not been realized in an actual solid. Recently however the Haldane model has been realized in a so called optical lattice using ultra cold fermionic atoms [26]. Despite being unrealistic in a solid state setting the Haldane model serves as a nice conceptual model to understand Chern insulators. Before we do so we should briefly discuss the properties of Chern insulators. As mentioned previously topological insulators can be put in different families depend on what symmetries they respect. A Chern insulator is a specific type of topological insulator where time-reversal symmetry is broken \(^2\). Time-reversal symmetry is satisfied if [22]

\[ THT^{-1} = H, \]

(3.2.9)

where \( H \) is single particle Hamiltonian in real space and \( T \) is the time-reversal operator. For spinless fermions this operator is given by \( T = U \mathcal{K} \) where \( U \) is some unitary operator and \( \mathcal{K} \) denotes the complex conjugation operator. The Chern insulator is characterized by the existence of gapless chiral edge modes. That is its edge states all propagate in the same direction. Therefore backscattering is impossible, even in the presence of impurities, since there is no state available with opposite chirality that an electron can scatter into. The chiral edge states therefore act as ideal one dimensional conductors. This has some striking consequences that we will discuss later in this chapter. In order to see that the Haldane model indeed describes a Chern insulator we will now investigate the topological properties of the model. As described in the previous section the topological properties of insulators are associated with the existence of a topological invariant. In order to study topological invariant we need to study the bulk of the system. Therefore we now consider the case where the two dimensional system has periodic boundary conditions. This allows us to write the Hamiltonian in Eq. (3.2.4) in momentum space. First we introduce the following operators:

\[ c_{k,\alpha} = \frac{1}{\sqrt{N}} \sum_j c_j e^{-ik \cdot r_j}, \quad c_{k,\alpha}^\dagger = \frac{1}{\sqrt{N}} \sum_j c_j^\dagger e^{ik \cdot r_j}, \]

(3.2.10)

where \( N \) is a normalization factor that denotes the number of sites on one sublattice and \( \alpha = A, B \) depending on what sublattice the site \( j \) resides on. The inverse transforms are given by

\[ c_j = \frac{1}{\sqrt{N}} \sum_k c_{k,\alpha} e^{ik \cdot r_j}, \quad c_j^\dagger = \frac{1}{\sqrt{N}} \sum_k c_{k,\alpha}^\dagger e^{-ik \cdot r_j}, \]

(3.2.11)

In momentum space the Haldane Hamiltonian takes on the following form:

\[ H_{\text{Haldane}} = \sum_k c_k^\dagger c_k \mathcal{H}(k) c_k, \]

(3.2.12)

where we defined the operators:

\[ c_k = (c_{k,A}, c_{k,B})^T, \quad c_k^\dagger = (c_{k,A}^\dagger, c_{k,B}^\dagger), \]

(3.2.13)

\(^2\)To the curious reader the Chern insulator belongs to symmetry class A, in the Altland-Zirnbauer classification scheme [23].
and the bulk Hamiltonian

\[ \mathcal{H}(k) = \epsilon(k)I + d(k) \cdot \sigma. \]  

(3.2.14)

Here \( I \) denotes the 2 × 2 identity matrix and \( \sigma \) is a vector containing the Pauli matrices. The remaining quantities are given by:

\[ \epsilon(k) = 2J_2 \cos(\phi) \left( \cos(k \cdot a_1) + \cos(k \cdot a_2) + \cos(k \cdot (a_1 - a_2)) \right) \]  

(3.2.15)

\[ d(k) = (d_1(k), d_2(k), d_3(k)) \]

\[ = \left( J_1 (1 + \cos(k \cdot a_1) + \cos(k \cdot a_2)), J_1 (\sin(k \cdot a_1) + \sin(k \cdot a_2)), M + 2J_2 \sin(\phi) (\sin(k \cdot a_1) - \sin(k \cdot a_2) - \sin(k \cdot (a_1 - a_2)) \right) \]  

(3.2.16)

The computational details for these results can be found in Appendix (A.1). To get the band structure we need to find the spectrum of the Haldane Hamiltonian. This is straightforward, we just need to diagonalize the bulk Hamiltonian in Eq. (3.2.14) for each \( k \). This is straightforward since we are dealing with a two band model. The spectrum for the Bulk Hamiltonian is given by

\[ E_{\pm}(k) = \epsilon(k) \pm |d(k)|. \]  

(3.2.17)

The energy bandgap between these bands is given by \( \Delta = 2|d(k)| \).

\[ \begin{align*}
\text{(a)} \\
\text{(b)}
\end{align*} \]

Figure 3.2: a) Bandstructure of the Haldane model. b) Spectrum around Dirac points \( K \) and \( K' \). The parameters used for both figures are \( J_1 = 1, J_2 = \frac{1}{2}, M = 0 \) and \( \phi = \frac{\pi}{35} \).

The bands are depicted in Fig. 3.2a. The parameters used are \( J_1 = 1, J_2 = \frac{1}{4}, M = 0 \) and \( \phi = \frac{\pi}{35} \). Generally as long as either \( M \) or \( \sin(\phi) \) are non-zero a bandgap will remain open. There are special areas where the gap is smaller then others corresponding to points where \( 2|d(k)| \) is smallest. Within the Brillouin zone of the Haldane model there are two such points. In the absence of the two last terms in Eq. (3.2.4) the gap closes and the spectrum is linear in momentum in the region around these points. These points are known as Dirac points and the area around each point is called the valley. Dirac points appear in many topological insulators. For instance they also appear when describing the surface of three dimensional topological insulators [5]. For the Haldane model the Dirac points are located at the points \( K = \frac{2\pi}{25}(1, \sqrt{3}) \) and \( K' = \frac{2\pi}{25}(1, -\sqrt{3}) \). In some cases a lot can be said about the physics of a model from the Dirac points and the surrounding region. As we discussed previously topological invariants can only change when a gap is closed or reopened somewhere. Therefore in order to study the topological properties of the Haldane model, we wish to study the part of the spectrum where a gap can close or open. The Dirac points are exactly the points where this happens. Therefore it is useful to expand the Hamiltonian around these points and use the result as an effective model. We now expand the Hamiltonian in Eq. (3.2.14) linearly around the points \( K \) and \( K' \).

\[ H_K = -3J_2 \cos(\phi) I + v_f (\sigma_x k_y - \sigma_y k_x) - \left( M - 3\sqrt{3}J_2 \sin(\phi) \right) \sigma_z, \]  

(3.2.18)

\[ H_{K'} = -3J_2 \cos(\phi) I - v_f (\sigma_x k_y + \sigma_y k_x) - \left( M + 3\sqrt{3}J_2 \sin(\phi) \right) \sigma_z. \]  

(3.2.19)
Here we introduced the Fermi velocity $v_f = \frac{3J}{2}$. Due to the linear $k$ dependence the spectrum is formally unbounded from above but of course this approximation is only valid up to a certain cutoff. We shall refer to these Hamiltonians as \textit{continuum Hamiltonians}. The term proportional to the identity in Eqs. (3.2.18-3.2.19) can be ignored since it only acts as a shift of energy in both bands. It is possible to write down a single continuum Hamiltonian which captures the physics of both valleys by introducing a valley subspace. The Hamiltonian then becomes a $4 \times 4$ matrix that takes the form:

$$H_{\text{continuum}} = v_f (k_y \sigma_x \otimes \tau_z - k_z \sigma_y \otimes I) - \sigma_z \otimes \left(M I - 3\sqrt{3} J_2 \sin(\phi) \tau_z \right),$$  \hspace{1cm} (3.2.20)

where the $\tau$ matrices denote the valley subspace and $\otimes$ denotes the tensor product. The spectrum of each valley is

$$E_K(k) = \pm \sqrt{v_f^2 (k_x^2 + k_y^2) + (M - 3\sqrt{3} J_2 \sin(\phi))^2},$$  \hspace{1cm} (3.2.21)

and

$$E_{K'}(k) = \pm \sqrt{v_f^2 (k_x^2 + k_y^2) + (M + 3\sqrt{3} J_2 \sin(\phi))^2}.$$  \hspace{1cm} (3.2.22)

These spectra are depicted in Fig. 3.2b.

### 3.2.1 Topological invariant and transport signatures in Chern insulators

To investigate the topological properties of the Haldane model we need to determine its topological invariant. For Chern insulators the relevant topological invariant is the Chern number \([2, 22]\). The Chern number of the $n$th band in a two dimensional Chern insulator is given by:

$$C_n = \frac{1}{2\pi} \int_{BZ} d^2k B_n(k),$$  \hspace{1cm} (3.2.23)

where the integral is over the two dimensional Brillouin zone and the quantity $B_n(k)$ is known as the Berry curvature of the $n$th band and it is given by \([22]\)

$$B_n(k) = i \left( \frac{\partial \psi_n(k)}{\partial k_x} \frac{\partial \psi_n(k)}{\partial k_y} - \frac{\partial \psi_n(k)}{\partial k_y} \frac{\partial \psi_n(k)}{\partial k_x} \right)$$  \hspace{1cm} (3.2.24)

where $|\psi_n(k)\rangle$ denotes the eigenstates of the $n$th band with crystal momentum $k$. The Chern number has a couple of important properties \([28]\). First of all it is known from mathematics that it can only assume integer values $^3$. Because it can only take on integer values the Chern number can only change discretely not continuously, as required of a topological invariant. Furthermore the Chern number of the $n$th band is the difference in the number of edge states above and below the $n$th band:

$$C_n = \chi_n - \chi_{n-1},$$  \hspace{1cm} (3.2.25)

where $|\chi_n\rangle$ denotes the number of edge modes in the gap below the $n$th band. The sign of the quantity $\chi_n$ depends on the chirality of the edge states which is set by the sign of the Chern number. This means that the Chern number can be negative as well if the edge modes in a given gap have negative chirality. In addition the sum of Chern numbers of all bands are always zero. In a non-driven system with $n$ bands the spectrum is bounded from below and also from above. Therefore there are no edge modes below the band with the lowest energy eigenstates and no edge modes above the band with the highest energy eigenstates. Consequently the number of edge modes in a given energy gap is simply the sum of the Chern numbers of all bands below that energy gap. These properties mean that the edge mode spectrum is determined from the Chern numbers of the bulk bands alone. This is an example of the Bulk edge correspondence that we mentioned in the beginning of this chapter.

We will now find a formula for the Chern number of the two bands in the Haldane model. Computing the Chern number directly by using eigenstates of the bulk Hamiltonian in Eq. (3.2.14) is a formidable task. If we assume that the Berry curvature is largest at the Dirac points and that it decays sufficiently fast away from these points, we may compute the Chern numbers using the Hamiltonian describing the valleys in Eq. (3.2.20) \([22]\). In Appendix (A.2) it is shown that for a Chern number of the valence band including the contribution from both valleys is given by

$$C = \left( \frac{\text{sign}(3\sqrt{3} J_2 \sin(\theta) - M)}{2} - \text{sign}(-M - 3\sqrt{3} J_2 \sin(\theta)) \right).$$  \hspace{1cm} (3.2.26)

$^3$In mathematics this is known as the Chern-Gauss-Bonnet theorem.
First we see that if we turn off the magnetic field the Chern number is always zero for all values of $M$. Secondly for a given $J_2$ and non-zero $\phi$ we will obtain a non-zero Chern number as long as $M$ is not too large. We observe that the equations $M = 3\sqrt{3}J_2 \sin(\theta)$ and $M = -3\sqrt{3}J_2 \sin(\theta)$ correspond to curves in the $(M, \phi)$ parameter space where the Chern number changes. In figure (3.3) the phase diagram of the Haldane model is depicted. The diagram is periodic along the $\phi$-direction so only one period of the diagram is depicted. We see that flipping the sign of $\phi$ also flips the sign of the Chern number. At particular values of magnetic flux different from zero the bandgap closes and the Chern number becomes zero. This happens at $\phi = \pm \pi$. This is due to the fact that these lead to the hopping parameters $J_2 e^{\pm i\pi} = -J_2$. At these particular values the hopping parameter is real not complex. This means that all the matrix elements of the Hamiltonian are real and therefore it respects time-reversal symmetry, therefore the Chern numbers have to be zero. Since the Haldane model has parameter regimes where the Chern number of each band is different from zero, it should have edge states in the spectrum in agreement with our discussion of the Chern number. However the Hamiltonian in Eq. (3.2.14) is a bulk Hamiltonian constructed for a system with periodic boundary conditions. In order to see edge modes emerge in the Haldane model we need to consider it in a finite geometry.

![Figure 3.3: Phase diagram of the Haldane model. This figure is a modified version of figure 2 in [6].](image)

Before we study a finite geometry we will briefly discuss an additional effect which occurs in Chern insulators as a consequence of their chiral edge modes namely the quantization of conductance in these systems. A common misconception is that insulators cannot conduct any current. This is in fact not completely true. The requirement is instead that insulators cannot dissipate energy. The power dissipated in an insulator is of the form $P \propto E \cdot J$, where $E$ is an external electric field and $J$ is the resulting current. Strictly speaking it is possible to have a non-zero current while still having no power dissipation. As long as the current is running perpendicular to the external electric field. The most general relation between $E$ and $J$ is

$$
\begin{pmatrix}
  J_x \\
  J_y 
\end{pmatrix} =
\begin{pmatrix}
  \sigma_{xx} & \sigma_{xy} \\
  \sigma_{yx} & \sigma_{yy}
\end{pmatrix}
\begin{pmatrix}
  E_x \\
  E_y 
\end{pmatrix}.
$$

(3.2.27)

The off diagonal component $\sigma_{xy} = -\sigma_{yx}$ is known as the Hall conductivity and it is insulators with non-zero Hall conductivity that can support a current. Chern insulators are an example of this. In fact not only do they posses a non zero Hall conductivity, but it is quantized in units of $\frac{e^2}{h}$. Not only is the Hall conductivity of a topological insulator quantized it is also incredibly robust to external perturbations such as disorder. This robustness comes from the topological properties of topological insulators. In fact the Hall conductivity of a Chern insulator at zero temperature is directly related to the Chern number: $\sigma_{xy} = \chi_n \frac{e^2}{h} C$, where $\chi_n$ are the number of modes in the energy gap where the Fermi energy is [22]. This quantization is similar to the one found by Thouless et al. for the integer quantum Hall effect (IQHE) of a two dimensional electron gas [2]. In fact the two systems belong to the same symmetry class and hence have the same topological invariant, namely the Chern number. For Chern insulators the integer quantum Hall effect appears without a net magnetic field however. There the quantization of Hall conductivity in Chern insulators has become known as the quantum anomalous Hall effect (QAHE). For this thesis however we will consider Chern insulators in transport settings. Here the measured quantity is conductance not conductivity. Therefore we will now introduce a physical picture that will help understand the conductance of Chern insulators in two terminal setups. The picture we will consider was first introduced by Büttiker [29]. Consider a clean two dimensional non-interacting Chern insulator of finite width connected to to two external leads with chemical potentials $\mu_1$ and $\mu_2$ respectively. If
the system is sufficiently long we can assume that crystal momentum is a good quantum number and that the wavefunctions of the system Hamiltonian consist of planewaves along the $x$-direction and some other function that depends on $y$. Although insulators are not perfect conductors the chiral edge modes present in Chern insulators do form perfectly conducting one dimensional channels due to the absence of backscattering. Therefore if we consider an energy window that only includes the gap. Now suppose the Chern insulator has $n$ different chiral edge modes. We now assume that the two chemical potentials differ by the voltage $\mu_1 - \mu_2 = -eV$ and that both chemical potentials are within the energy window considered. The current through a single channel can be found as $I = -e \int_{\mu_2}^{\mu_1} v(\mathcal{E})\rho(\mathcal{E})$, where $-e$ is the electron charge, $\rho(\mathcal{E})$ is the density of states in one dimension and $v(\mathcal{E})$ is the electron velocity. In one dimension the density of states is given by \[ \rho(E) = \frac{1}{2\pi\hbar v(E)}. \] The current therefore becomes $I = -n\frac{e}{h}(\Delta\mu)$, where $n$ is the number of channels. In the scenario described above the conductance is therefore

$$G = n\frac{e^2}{h}. \quad (3.2.28)$$

This result is quite universal in the sense that we didn’t have to assume anything specific about the edge mode dispersion or the material of interest. The same argument can be applied to the IQHE and reflects the universality of the quantum Hall effect [29].

### 3.2.2 Edge modes in the Haldane model

To study edge modes we consider the Haldane Hamiltonian in the ribbon geometry depicted in figure (3.4). In this geometry the system has translational invariance in one direction only, while being finite in the other direction. The system therefore has two edges. For a hexagonal lattice there exist several types of edge configurations [27]. Here we focus on the zig-zag configuration.

![Ribbon geometry for a hexagonal lattice with zig-zag edges. The strips are the collection of sites encircled by oval rings.](image)

Although a two unit cell is not possible it is useful to define so called strips. That is one dimensional chains that run across the finite direction. These can be thought of as the new unit cell for the ribbon geometry. When we wish to analyze this new system it is therefore useful to label sites according to their slice and what lattice site on the slice they reside on. A Fourier transform can still be defined along the direction with translational invariance. Here we choose this direction to be the $y$-direction. The Hamiltonian still contains the site index, so the size of the Hamiltonian considered will depend on the
strip length. In Appendix A.3 it is shown that the Hamiltonian takes the form

\[ H_{\text{ribbon}} = 2J_1 \sum_{k_y} \sum_{j=1}^{L/2} \left( c_{2j, k_y}^\dagger c_{2j+1, k_y} + \text{h.c.} \right) + J_1 \sum_{k_y} \sum_{j=1}^{L-1} \left( c_{2j, k_y}^\dagger c_{2j+1, k_y} + \text{h.c.} \right) \]

\[ + \sum_{k_y} \sum_{j=1}^{L/2} \left( c_{2j-1, k_y}^\dagger c_{2j-1, k_y} \left( M + 2J_2 \cos(\sqrt{3}k_y) \right) - c_{2j, k_y}^\dagger c_{2j, k_y} \left( M - 2J_2 \cos(\sqrt{3}k_y) \right) \right) \]

\[ + 2J_2 \sum_{k_y} \sum_{j=1}^{L/2-2} \left( c_{2j, k_y}^\dagger c_{2j+2, k_y} \cos(\sqrt{3}k_y) + \text{h.c.} \right) \]

\[ + 2J_2 \sum_{k_y} \sum_{j=1}^{L/2-2} \left( c_{2j-1, k_y}^\dagger c_{2j+1, k_y} \cos(\sqrt{3}k_y) + \text{h.c.} \right). \]  

This Hamiltonian has to be diagonalized numerically for each value of \( k \). We have done so in two parameter regimes, first in the topological regime where \( C = 1 \) and then in the trivial regime where \( C = 0 \). In Fig. 3.5a the Hamiltonian has been diagonalized in the topological regime with parameters: \( J_1 = 1, J_2 = \frac{1}{4}, \phi = \frac{\pi}{2} \) and \( M = 0 \). In Fig. 3.5b as well as in the trivial regime with parameters: \( J_1 = 1, J_2 = \frac{1}{4}, \phi = 0 \) and \( M = 1 \). In Fig. 3.5a we see that two gapless chiral edge modes emerge. This makes sense since the ribbon has two edges and the Chern number predicts one mode pr. edge. The states have opposite group velocity \( v = \frac{\hbar}{\pi} \frac{\partial E}{\partial k_y} \) meaning they propagate in opposite direction on opposite edges. It is straightforward to verify that the topological edge modes in Fig. 3.5a are indeed localized at the edge. In Fig. (3.6a) the wavefunctions of the topological edge states at momentum \( k_y = 0 \) are depicted for both edges. We see that the wavefunctions are indeed localized at the edges as they should be. In Fig. 3.5b we see the spectrum in the trivial regime. Here no gapless modes emerge. However we do see states at \( E = 1 \) and \( E = -1 \) with a constant energy as a function of \( k_y \). These states are in fact localized at the edge but are not topological states and occur only due to the zig-zag boundary of the ribbon. Furthermore these states have velocity zero meaning they are not propagating along the edge like the topological edge modes in Fig. 3.5a.

![Figure 3.5: a) Bandstructure in the topological regime, with \( J_1 = 1, J_2 = \frac{1}{4}, \phi = \frac{\pi}{2} \) and \( M = 0 \). b) Bandstructure in the trivial regime with \( J_1 = 1, J_2 = \frac{1}{4}, \phi = 0 \) and \( M = 1 \). Each strip on the ribbons used for both simulations contain 300 sites.](image)

The ribbon geometry is useful because it gives a numerical solution for a system of finite size and therefore allows the study of edge modes. However it is also possible to reveal more general features of the edge states from a toy model that can be solved analytically. The bulk-boundary correspondence dictates that edge states have to exist at the boundary between two topologically distinct Hamiltonians. To see how this argument applies to the Haldane model we now imagine a setting where two topologically
distinct regions are put together at $x = 0$. Each region extends from $x = 0$ to $\pm \infty$ and far away from the edge at $x = 0$ the materials are well described by a bulk Hamiltonian. In this system translational invariance is maintained along the $y$-direction. Suppose that the bulk material on each side of the interface are Chern insulators described by the Haldane model. For the Haldane model we saw that the linearized Hamiltonian captured the essential physics by predicting the emergence of edge modes. However in this geometry both crystal momenta are not good quantum numbers. However we can still study the system in real space. The real space representation of momentum is $p = -i\hbar \nabla$. A natural guess at a Hamiltonian that reproduces the continuum model of a single valley in Eq. (3.2.19) is therefore:

$$H_{\text{Dirac}} = -v_f \left( i\hbar \frac{\partial}{\partial x} \sigma_y + i\hbar \frac{\partial}{\partial y} \sigma_z \right) + m(x)\sigma_z.$$  

(3.2.30)

For a system with translational invariance the eigenstates can be taken as plane waves and it is straightforward to verify that the first two terms in Eq. (3.2.30) reproduce the terms linear in momentum in Eq. (3.2.20). The physical nature of the final term might seem less obvious. The final term is a mass term that makes the model topological. If we compare with the linearized Haldane Hamiltonian the term would be $J_23\sqrt{3}\sin(\phi)$. The mass term has to change sign in order for the phases to differ. Let $m(x) > 0$ for $x > 0$ and $m(x) < 0$ for $x < 0$. For two topological insulators described by the Haldane model this would correspond to the case where the magnetic flux is different from zero both has opposite sign in each insulator. The only length scale in the problem is the mass term $m(x)$, therefore the solution must dependent on this function alone.

(a)  
(b)

![Figure 3.6](image-url)

Figure 3.6: a) Numerical obtained edge states for the same system as Fig 3.5a. As predicted from the bandstructure there are is one edge state pr. edge. They both decay rapidly as the bulk is approached b) Normalized solutions edge mode model in Eq. (3.2.34) with the topological mass $m_0 = 1$ and $m_0 = 10$ corresponding to the localization lengths $\xi = 5$ and $\xi = 1$ respectively. Here we set $\hbar = 1$ and $v_f = 1$.

Given the numerical results we have seen and our discussion of the bulk-edge correspondence, we expect to find a localized wavepacket at the boundary. Furthermore we require that the wavefunction vanishes at $\pm \infty$. Since all terms depend on only one coordinate we can use separation of variables. The spinor solution can therefore be written as

$$\Psi(x, y) = \begin{bmatrix} \phi_1(x) & \phi_2(x) \end{bmatrix}.$$  

(3.2.31)

Due to translational invariance in the $y$-direction, the wavefunctions $\phi_1(y)$ and $\phi_2(y)$ are plane waves: $\exp(-ik_y y)$. The spinor solutions may then be written as:

$$\Psi(x, y) = e^{-ik_y y} \begin{bmatrix} \phi_1(x) \\ \phi_2(x) \end{bmatrix}.$$  

(3.2.32)

For a normal Dirac Hamiltonian without a mass term $m(x)$ the dispersion is linear in momentum. This is the case around the $x = 0$ region where the mass changes sign. Furthermore we saw that the edge
states we obtained numerically had linear dispersion. Therefore it seems plausible to look for solutions where \( E = \hbar v_f k_y \). In Appendix A.4 we show that this leads to solutions of the form:

\[
\Psi(x, y) = \chi(x, y) \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \quad \chi(x, y) = \frac{1}{\sqrt{C}} e^{i k_y y - \frac{\hbar}{\tau} f^e dx' m(x')}, \tag{3.2.33}
\]

here \( C \) is a normalization constant. We are able to make two observations from the analytic solution. The solution contains plane waves that propagate with velocity \( v_f \) along the interface boundary. Therefore they all have a specific chirality like we discussed previously. Furthermore the solution is localized at the boundary at \( x = 0 \) and decays exponentially with the distance away from the boundary, in agreement with the numerical results for the ribbon. The localization happens on a length scale set by the topological mass term \( m(x) \). This last observation is important since it relates the size of the gap in the bandstructure of the bulk to the localization length of the edge mode solution. For a given mass term \( m(x) \) the solution will be localized within a length \( \xi = \frac{\hbar v_f}{m_0} \), where \( m_0 \) is the size of \( m(x) \) inside either of the two materials. A good example of a mass term that satisfies the conditions above would be \( m(x) = m_0 \tanh(x) \). This corresponds to a mass term that changes sign at the boundary and then saturates at the value \( -m_0 \) and \( m_0 \) in the bulk of the two topologically distinct materials. In this case the wavefunction \( \chi(x, y) \) of the edge state becomes

\[
\chi(x, y) = \frac{1}{\sqrt{C}} e^{i k_y y} (\cosh(x))^{-\frac{\hbar}{v_f} \xi}, \tag{3.2.34}
\]

where the parameter \( \xi \) is the localization length of the state given by \( \xi = \frac{\hbar v_f}{m_0} \). The normalized solution has been plotted in Fig. 3.6b for two different sizes of \( m_0 \). We see that in order for the edge states to remain localized the mass must be large. In a finite system with width \( W \) the localization length must satisfy \( W \gg \xi \) in order for an edge state to remain localized at one edge. If not it is possible for the edge state to tunnel from one edge to another. The fact that the localization length is inversely proportional to the topological mass is a general feature of topological insulators and plays an important role when these systems are considered in transport settings. The localization length of edge states will be important when we pick parameters for numerical simulations of finite systems later in the thesis.

### 3.3 Floquet Topological Insulators

Despite the interesting features of the Haldane’s model, it does not describe any known solid state realization of a Chern insulator. Not long ago however it was suggested that topological insulators can be created by applying a external drive that is periodic in time. Specifically a non-equilibrium model which is an analog of the equilibrium Haldane model has recently been suggested [7]. It was theoretically predicted that by shining circularly polarized light onto a graphene sample, from above, would produce a Chern insulator and that a quantized Hall response could be observed [7, 9].

The system is described by the Hamiltonian:

\[
H(t) = \sum_{ij} \left( J_{ij}(t) c_i^\dagger c_j + h.c. \right), \tag{3.3.1}
\]

where the dynamical hopping parameter is given by

\[
J_{ij}(t) = J_1 e^{i A_{ij}(t)}, \tag{3.3.2}
\]

where \( A_{ij}(t) \) is the component of the magnetic vector potential along the \( r_{ij} \) bond and it is given by \( A_{ij}(t) = (-\frac{\hbar}{\tau}) A(t) \cdot (r_j - r_i) \). The light has circular polarization such that time reversal symmetry is broken like it was in the Haldane model. In this case the magnetic vector potential is given by \( A(t) = A_0 (\cos(Î‡t), \rho \sin(Î‡t)) \), where \( A_0 \) is the amplitude and \( \rho = \pm 1 \) determines whether the drive has left or right circular polarization. The electric field corresponding to this magnetic vector potential is \( E(t) = -\frac{\partial A(t)}{\partial t} \). Therefore the magnitude of the magnetic vector potential is \( A_0 = \frac{E_0}{\hbar} \), where \( E_0 \) is the electric field amplitude. To analyze the model we now impose periodic boundary conditions such that we can find a bulk Hamiltonian for the model in Eq. (3.3.1). This model is equivalent to the nearest neighbor term introduced in (3.2.5). For now we will only be interested in the linearized part obtained in Eq. (3.2.20). In the continuum model it is straightforward to add the external drive. It enters by minimal coupling: \( k \to k - \frac{e}{\hbar} A(t) \). The continuum version of equation Eq. (3.3.1) is therefore

\[
H(t) = v_f \left( \left( k_y - \frac{e}{\hbar} A_y(t) \right) \sigma_x \otimes \tau_z - \left( k_x - \frac{e}{\hbar} A_x(t) \right) \sigma_y \otimes I \right). \tag{3.3.3}
\]
To get a complete understanding of the model we will need to consider the full lattice model, however it is to difficult to analyze analytically so we will postpone this till later in the chapter. Instead we will focus on trying to understand the linearized model to see how periodic driving can be used to generate a Chern insulator. The cases of off- and on resonant driving frequencies will be discussed seperately.

### 3.3.1 Off-resonant driving frequencies

In order to understand why the Hamiltonian in Eq. (3.3.3) describes a Chern insulator it is useful to look at the model in the high frequency limit. In this limit the system is subject to a rapidly oscillating driving field and the system dynamics are well captured by studying the time evolution over a single period [30]. The time evolution of the system over a single period is captured by the time evolution operator:

\[ U(T) = T e^{-i \int_0^T dt H(t)}, \]

where \( H(t) \) is the Hamiltonian of the system and \( T \) denotes the time-ordering operator. In the literature of periodically driven systems this particular time evolution operator is known as the Floquet operator. In the case where the dynamics on long timescales are well captured by the time evolution within one period of time it is useful to define an effective Hamiltonian. The effective Hamiltonian is defined as [30]

\[ H_{\text{eff}} = \frac{i}{T} \ln(U(T)). \]

It is not always possible to obtain an effective Hamiltonian for a generic periodically driven system [30]. But for non-interacting systems it is possible to perform a high-frequency expansion to obtain an expression for \( H_{\text{eff}} \). Such an expansion is only convergent when the driving frequency is sufficiently large. Typically it is sufficient that \( \hbar \Omega \) is the largest energy scale in the problem. For the model considered here it is sufficient that \( \Omega \gg J_1 \). The number of terms one needs to keep in this expansion depends not only on the frequency but also on the driving amplitude. It can shown that this expansion is equivalent to treating the problem using time-dependent perturbation theory [30]. If we focus on high-frequencies and small driving amplitudes it is sufficient to keep first order corrections only. For the graphene model in Eq. 3.3.3 it was shown that the corresponding effective Hamiltonian to first order in the high frequency expansion becomes [9]

\[ H_{\text{eff}} = v_f (k_y \sigma_y \otimes \tau_z - k_x \sigma_x \otimes I) \pm \sigma_z \otimes \tau_z \frac{v_f A^2}{\hbar \Omega} \]

where \( A = \frac{\hbar a A_0}{\hbar} \), \( a \) is the lattice constant of graphene and it is assumed that \( A^2 \ll 1 \). The first part is just the linearized version of the Hamiltonian without an external drive. The second part is a term that opens a gap in the spectrum. Since the driving frequency is much larger than the actual bandwidth of the system, there is no single particle states in the two bands that are connected by an energy difference of \( \hbar \Omega \) and therefore the electrons cannot directly absorb photons. It is however possible to have higher order processes where a single electron absorbs and then emits the same number of photons and vice versa. Due to the drive being circular there is a phase difference between these two processes. In fact it is these virtual photon absorption-reemission processes that give rise to the term \( \pm \sigma_z \otimes \tau_z \frac{v_f A^2}{\hbar \Omega} \). Effective Hamiltonians are time-independent Hamiltonians. Therefore it is possible to analyze their topological properties by applying the same analysis we used for the Haldane model. By directly comparing the result Eq. (3.3.6) with the linearized version of the Haldane model obtained in Eq. (3.2.20) we see that the two Hamiltonians are structurally similar. However the parameters have a different physical origin. The topological term in the Haldane model is \( J_2 \sqrt{3} \sin(\phi) \). For the driven model above the gap opening term is \( \frac{v_f A^2}{\hbar \Omega} \). The Haldane model has an on-site potential term. This term is however not necessary since the important term is the one that breaks time-reversal symmetry. For the periodically driven model the gap size is essentially set by the fraction \( \frac{A^2}{\hbar \Omega} \). Except for the difference in origin the effective Hamiltonian has the same topological properties and therefore describes a Chern insulator. The circularly polarized drive corresponds to the two points in the phase diagram of the Haldane model where \( \phi = \pm \frac{\pi}{2} \), where the sign is determined from the chirality of the drive (left/right polarization). This puts the driven model in the topological phase where the Chern number of the lower band is \( C = \pm 1 \). The external drive can not only induce a topological gap. It can also control the sign on the Chern number, which means it can control the chirality of the emerging chiral edge modes. Since the driving frequency has to be high and the driving amplitude has to be small the fraction \( \frac{A^2}{\hbar \Omega} \) will be small and so will the bandgap. This makes
the edge states in the high frequency limit difficult to detect experimentally. Furthermore the toy model we present here only has two bands. Real materials however have many different bands. Therefore in reality even at high frequency there can be higher bands that electrons can access by absorbing photons. Therefore a high driving frequency no longer guarantees the off-resonance condition. Due to these issues it is desirable to create a gap using a lower frequency. When the frequency becomes sufficiently low we reach the on-resonance limit and we have to analyze the problem differently.

3.3.2 On-resonant driving frequencies

In light of the disadvantages of the high-frequency limit, a natural question to ask is if topological gaps can also be obtained at low frequencies where the driving frequencies are comparable to or within the bandwidth of the driven system. To answer this question we return to the Hamiltonian in Eq. (3.3.3). To make things simpler the following analysis is done for one valley only. However the same analysis can be done for the valley we neglect here. For this part of the analysis we choose the light polarization such that the vector potential is $A(t) = A_0 \left( \cos(\Omega t), -\sin(\Omega t) \right)$. We will now apply the extended space formalism we introduced in section 2.2. Because we are working with the linearized model the extended space Hamiltonian becomes block diagonal

$$H_{EZ} = \begin{pmatrix} \vdots & \vdots & \vdots & \vdots \\ \cdots & H_0 + \Omega & H_1 & 0 \\ \cdots & H_1 & H_0 & \cdots \\ 0 & H_1 & H_0 - \Omega & \cdots \\ \vdots & \vdots & \vdots & \cdots \end{pmatrix}. \quad (3.3.7)$$

Here each block has dimension $2 \times 2$. It is sufficient to truncate this extended space onto a $4 \times 4$ subspace to capture the physics at weak driving amplitude. In Appendix A.5 it is shown that the truncated Hamiltonian becomes

$$H_{EZ} = \begin{pmatrix} \hbar \Omega \over 2 & \hbar v_f k_- & 0 & 0 \\ \hbar v_f k_+ & \hbar v_f A_0 & 0 & 0 \\ 0 & \hbar v_f A_0 & \hbar v_f k_- & 0 \\ 0 & 0 & \hbar v_f k_+ & \hbar \Omega \over 2 \end{pmatrix} + \hbar \Omega \over 2 I. \quad (3.3.8)$$

We now consider the truncated Hamiltonian in Eq. (3.3.8) in the case where the external drive is turned off ($A_0 = 0$). Here the two subspaces are completely decoupled and the system is described by $H_0$. The system just has two bands, a valence band and a conduction band, see Fig. (3.7a). When extended space is introduced the system has to copies of the original Hamiltonian: $H_0$ and $H_0 + \Omega$. The last component is identical to the first but simply produces quasi energies that are shifted $\epsilon' = \epsilon + \Omega$. In Fig. (3.7b) the quasienergy bands of $H_0$ as well as the copy of the lower band are depicted. The quasienergy spectrum is degenerate at $E = \hbar \Omega \over 2$ for $k = k_0$, where $k_0 = \frac{2v_f}{\hbar \Omega}$. For a finite driving amplitude $A_0$ on the drive couples the two subspaces together which effectively leads to a hybridization between the $m = 0$ conduction band and the $m = 1$ valence band. This hybridization lifts the degeneracy at $E = \hbar \Omega \over 2$ and opens a gap as seen in Fig. (3.7c). For the plots we used the parameters $J_1 = 1$, $\Omega = 3$ and for the final plot $\eta = 0.15$, where $\eta = \frac{e v_f A_0}{\hbar \Omega}$. 

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Figure 3.7: a) The linear Dirac dispersion of the non-driven model. The blue band represents the valence band and the red band the conduction band. b) A visualization of the four bands in extended space without any external drive. For the truncated picture we have included the $m = 0$ conduction and valence band as well as the $m = 1$ copy of the conduction band and also valence band which now overlaps with the $m = 0$ conduction band. c) The $m = 1$ valence band has hybridized with the $m = 0$ conduction band to create two new bands with a gap in between.

In Appendix (A.5) it is shown that the quasienergy spectrum near the degenerate points for a weak driving field becomes:

$$
\epsilon_{\pm} = \frac{\hbar \Omega}{2} \left( 1 \pm \sqrt{\left( 1 - \frac{k}{k_0} \right)^2 + \eta^2} \right),
$$

(3.3.9)

where $k = \sqrt{k_x^2 + k_y^2}$. The size of this resonant gap is:

$$
\Delta_1 = \hbar \Omega \eta = e v_f A_0.
$$

(3.3.10)

This gap scales only linearly with $A_0$ unlike the off-resonant result which scales as quadratically with $A_0$. Therefore the size of the dynamical gap will be much larger in the weak driving limit. This method overcomes the issues previously mentioned. This way of opening a gap by mixing different bands applies not just to the toy model presented here but is a generic mechanism for producing a gap in periodically driven systems [8]. It is similar to the band-inversion mechanism that was originally proposed to create an equilibrium topological insulator [3]. It is even possible to extend the idea to multi-photon resonances. That is frequency regimes where $D \gg n \Omega$, where $D$ is the bandwidth of the model in consideration and $n$ is an integer larger than one. This can for instance be applied to materials that unlike graphene are gapped without an external drive. It is then possible to find a small driving frequency, such that the energy $\hbar \Omega$ is too small to excite an electron from the valence band into the conduction band. If however the energy of absorbing two photons $2\hbar \Omega$ is enough to achieve resonance, this can instead lead to topological gap opening. This is known as a two-photon resonance [31].

So far we have only discussed linearized models. While these models are excellent to build an intuition for the driven model in Eq. (3.3.1) a treatment of the full bandstructure is necessary to make precise predictions. Furthermore so far we have only studied bulk Hamiltonians. To see edge states emerge we need to study the Hamiltonian in Eq. 3.3.1 in a finite geometry like we did for the non-driven...
model. Instead of starting from square one we choose an approach similar to what we did for the non-driven Haldane model. That is we study the graphene model in a ribbon geometry with zig-zag edges. Here \( k_y \) is still a good quantum number and the decomposition of creation and annihilation operators into new momentum resolved operators is similar to what was done in Appendix A.3. The Hamiltonian is now time-dependent however. In order to predict the quasienergy spectrum we therefore apply the extended space formalism introduced in section 2.2. Because we consider the full lattice the extended space Hamiltonian is no longer block diagonal. A detailed analysis of how to obtain this Hamiltonian is given Appendix A.6. There it is shown that the \( n \)’th harmonic of the Hamiltonian becomes

\[
H_n = J_1 \sum_{k_y} \sum_{j=1}^{\frac{L}{2}} \left( 2 \cos \left( \frac{\sqrt{3}}{2} k_y a - n \rho \frac{2 \pi}{3} \right) e^{i n \rho \frac{2 \pi}{3}} J_{n \rho} (\lambda) c_{2j, k_y}^\dagger c_{2j+1, k_y} + 2 \cos \left( \frac{\sqrt{3}}{2} k_y a + n \rho \frac{2 \pi}{3} \right) e^{i n \rho \frac{2 \pi}{3}} J_{n \rho} (-\lambda) c_{2j, k_y}^\dagger c_{2j+1, k_y} \right) + J_1 \sum_{k_y} \sum_{j=1}^{L-1} \left( c_{2j, k_y}^\dagger c_{2j+1, k_y} i^{-n} J_{-\lambda} (\lambda) + c_{2j, k_y} c_{2j+1, k_y}^\dagger i^{-n} J_{-\lambda} (-\lambda) \right),
\]

(3.3.11)

where we defined the effective hopping parameter \( J_{p(\omega)} (\lambda) = J_0 J_{p(\omega)} (\lambda) = \frac{\pi a}{\xi} \). To analyze the spectrum of the extended zone model we need to solve it numerically. This has been done using an extended space with dimension \( n \times (2M + 1) \) where \( M = 3 \) and \( n = 300 \), \( n \) being the number of lattice sites used. We used the system and drive parameters: \( J_1 = 1, \Omega = 3, \lambda = 0.5, \rho = 1 \). In Fig. 3.8a the resulting quasienergy spectrum is depicted. We see gapless edge states appear at each edge in the dynamical gap. Furthermore we see that taking into account several copies leads to a gap at \( E = 0 \). This gap was simply absent because only two copies were kept in the analysis of the on-resonant case. This is because the photon-absorption reemission processes are still present. They are however second order processes and for weak driving the dynamical gaps will be larger as discussed previously. We see that the dynamical gap \( \Delta_1 \) has two modes pr. edge. It has been verified that the two modes at one edge in the \( E = \frac{\pi a}{\xi} \) have opposite chirality of the mode in the \( E = 0 \) \cite{27}. In addition to obtaining the full spectrum the lattice model also reveals a feature not captured by the linearized Hamiltonian. That is the hopping parameter \( J_1 \) becomes modified by the drive such that the new effective hopping parameter is \( J_{\text{eff}} = J_0 (\lambda) = J_0 J_{\omega(0)} (\lambda) \). This has the physical consequence that the new bandwidths are smaller compared to those of the non-driven graphene sheet. It is important because the bandwidth is what we compare the driving frequency to. Therefore although graphene has a bandwidth \( D = 6 \) (for \( J_1 = 1 \)) and we used \( \Omega = 3 \) we are still only capturing the one photon resonance and not the two-photon resonance. Because for the parameters used here the effective hopping parameter is \( J_{\text{eff}} \approx 5.63 \). For experimental purposes the driving intensities used are too small for this to be a significant effect in solid state settings, but it is something that one has to be aware of. It is important to emphasize that one should only count the lower part of the modes in the \( E = \frac{\pi a}{\xi} \) gap and the upper part of the modes in the \( E = -\frac{\pi a}{\xi} \) gap since these connect due to the periodicity of the quasienergy.

The creation of topological states using circularly polarized light has been achieved experimentally. They were observed in an experiment on the 3D material Bi₂Se₃ which is a topological insulator. The 2D surface of this material is well described by a single Dirac cone. The circularly polarized drive was then used to drive the material into a topological phase. The Floquet-Bloch bands were obtained in analogy to what is done for non-driven systems. In non-driven systems bands can be mapped out using a technique called ARPES (Angled-resolved-photoemission-spectroscopy). For a driven system the concept is the same except the time scales on which the bands are observed are important and depend on the driving period. For this reason an ARPES measurement with a good time-resolution is needed. Therefore this technique is known as TrARPES (time-resolved-angle-resolved-photoemission-spectroscopy). This experiment was performed by the group lead by N. Gedik at MIT \cite{32}. Their result is depicted in Fig. 3.8b. The figure shows the quasienergy bands of a 3D topological insulator projected onto the crystal momenta \( k_x \) and \( k_y \) respectively. The colors indicate intensity of the measured signal. Despite the success of this experiment the nature of the edge states in Floquet topological insulators is slightly different from those in static topological insulators. Which we will now address.
Figure 3.8: a) Floquet-Bloch bands for full the model in Eq. (3.3.1) in a ribbon geometry. The quasienergy spectrum is projected onto $k_y$. For this plot the following parameters where used $J_1 = 1$, $\Omega = 3J_1$ and each strip contains 300 sites. b) Floquet-Bloch bands of the surface of periodically driven Bi$_2$Se$_3$. The different $n$’s indicate different sidebands. The picture is taken from [32].

3.3.3 Differences between periodically driven and non-driven topological systems

Topological insulators out of equilibrium distinguish themselves from their non-driven counterpart in many ways. In section 3.2.1 it was demonstrated that for the non-driven Chern insulator the Chern numbers of all the bands was enough to fully predict the edge mode spectrum. It turns out that establishing a bulk-edge correspondence for Floquet topological insulators is not straightforward at all. It has been shown that an additional topological invariant must be found and computed in order to successfully predict the number of edge states in a given gap [33]. This anomalous behavior is due to the fact that Floquet-Bloch bands are formed by quasienergy and not energy. As explained in Chapter 2 quasienergy is a periodic quantity which enables new types of bandstructures which are impossible in non-driven systems. To illustrate this concept we consider the bandstructure in Fig 3.8a once more. This bandstructure has new features namely we see gapless modes in the gap at $E = \hbar \Omega/2$ which stop at the boundary of the Floquet Brillouin zone and then reappear in the gap at $E = -\hbar \Omega/2$ where they connect to a bulk band. Such states are perfectly allowed in driven systems due to the periodicity of the quasienergy. It is still possible to compute Chern numbers of the quasienergy bands but their properties will no longer be enough to successfully determine if edge modes appear. As mentioned the Chern number only counts the difference in edge states above and below a given band. For a non-driven topological insulator we know that the lowest band in a given model cannot have an edge state connected below. The same argument applies to the band with the highest energy, which can’t have edge modes with energies above the band. In a periodically driven topological insulator it is possible that the Chern numbers of all bands are zero, and that gapless edge modes still exist in the bandgaps, as long as the number of edge states in each gap is the same [33]. As such the Chern number is still well defined, it is just that it no longer suffices to establish a bulk-edge correspondence in driven systems. These edge modes are known as anomalous edge states and they are a unique feature of Floquet topological insulators. Despite this subtlety a complete topological classification of Floquet-Bloch bands has been given [34]. In addition to the difference in topological nature there is also a difference between the edge modes of driven and non-driven systems. For a non-driven topological insulator the edge state is a stationary state. This means that if it is localized at the edge at one time it will continue do be so for all times. In a driven systems the eigenstates of the Floquet Hamiltonian are Floquet states. This also goes for the edge states. Therefore it is natural to ask if the Floquet edge states remain at the edge at all times. We know that the Floquet states are periodic in time. This means that if a wavepacket is localized at the edge at one time it will also be localized at $t + T$. However we can imagine that a wavepacket can move around during the period and then return to the original configuration at time $t + T$. A natural question to ask is if Floquet edge states really are edge states. There are several ways to address this problem. In one
of the first papers written on this subject it was shown by direct numerical computation that the edge
states in the toy model for a Floquet topological insulator were well localized at all times [8]. Another
way is to make an analytic toy model for edge states similar to what was done in section 3.2.2. This has
in fact been done for the graphene system considered here and they are in good agreement with what
was observed numerically [27]. More generally the edge states cannot travel further than the distance
cT, where c denotes the speed of light and T the period of the drive. For non-relativistic particles a
more rigorous statement can be made using so called Lieb-Robinson bounds [35]. Such bounds are upper
bounds on how fast information can propagate. Therefore in reality it is enough to consider such bounds.
Although a small deformation of the wavepacket is possible one can always consider a system with a
width that exceeds the distance the wavepacket is allowed to travel by the Lieb-Robinson bound.

In addition to the existence of edge states in the model above, it is natural to ask if Floquet topo-
logical insulators also exhibit a quantized Hall response. So far no clear definitive experimental signature
has been observed. Recently however an experiment conducted in the group of A. Cavalleri found some
signatures which could be interpreted as robust Hall currents [36]. The measured conductance was not
quantized in units of $\frac{e^2}{h}$. There are several possible explanations for this deviation. In this thesis we
address one of these issues namely photon assisted tunneling. To understand that this is an issue we
consider a transport setup similar to the one presented in section 3.2.1. Here we argued that as long
as a small bias is present and that the chemical potentials reside in the gap a quantized conductance is
obtained. Unlike the non-driven systems electrons can now absorb photons from the driving field while
inside the Floquet topological insulator. In Fig 3.9a this scenario is depicted. For simplicity the picture
contains only a single energy level in the gap, which may be interpreted as a particular edge state. In the
presence of a periodic drive an edge state can absorb a photon thereby causing the electron occupying
the state to end up in the conduction band and exit the system into the second lead. In this case the
transport process is not mediated by an edge state alone and therefore there is no reason to expect a
quantized response. To circumvent this issue a recent proposal was to insert additional leads, in between
the system and the wide band leads, with a narrow bandwidth. We refer to such narrow bandwidth
leads as energy filtered leads. If these energy filtered leads have a bandwidth $D_f < \hbar \Omega$ an electron won’t
be able to absorb a photon and subsequently exit into a lead since it has to go through the energy filter
first. This scenario is depicted in Fig. 3.9b.

![Figure 3.9: a) Transport through a periodically driven system with wide band leads. The transport is
not mediated by an edge state alone since the electron absorbs a photon from the drive ending up in a
bulk state. b) Transport through a periodically driven system with narrow band leads inserted. Photon
absorption processes are suppressed because electrons can only exit the system within the small energy
window they used to enter the system.](image)

In order to analyze transport through Floquet topological insulators we first need to develop a general
framework that will allow us to describe transport in periodically driven systems.
Chapter 4

Transport and physical observables in periodically driven quantum systems

In this chapter a general formalism to study transport through periodically driven systems is introduced. First a simple two terminal setup is introduced. Subsequently an equation for the current through this configuration is found. It is argued that the current can be expressed in terms of non-equilibrium Green’s functions. The Keldysh formalism is briefly introduced and used to obtain non-equilibrium Green’s functions. These are in turn used to derive the well known Jauho Wingreen Meir formula. This result is used to show that the steady state current through periodically driven non-interacting systems is described by a Floquet analogue of the well known Landauer-Büttiker formula for non-driven, non-interacting systems. Finally it is shown how other relevant quantities such as time-averaged density of states, particle density, local current and non-equilibrium distribution functions can also be obtained using Green’s functions. Throughout this chapter only spinless particles are considered.

4.1 Transport in two terminal configurations

A central theme in mesoscopic physics is the question of how to compute the current through a mesoscopic region with external leads attached. The most simple transport setup imaginable is the two terminal configuration which consists of a system connected to two contacts which are modeled as two fermionic particle reservoirs. The Hamiltonian for this setup is given by

\[ H(t) = H_S(t) + H_t + H_c, \]

where we have defined a Hamiltonian for the system \( H_S(t) \), one for the leads \( H^c \) and a Hamiltonian that describes tunneling between system and leads \( H_t \). These Hamiltonians are given by

\[ H_S(t) = \sum_{mn} h_{mn}(t) d_m^\dagger d_n, \quad H_c = \sum_{\alpha \in L,R} \epsilon_{\alpha} c_{\alpha}^\dagger c_{\alpha}, \]

\[ H_t = \sum_{\alpha,m} V_{\alpha,m}^* d_m^\dagger c_{\alpha} + V_{\alpha,m} c_{\alpha}^\dagger d_m, \]

where the Hamiltonian’s in bold letters denote matrices. The vectors are defined as:

\[ d = (\cdots d_m \cdots)^T, \quad c = (\cdots c_{\alpha} \cdots)^T, \]

where the vector components \( d_m \) and \( c_{\alpha} \) denote fermionic annihilation operators for the \( m \)’th site in the system and the \( \alpha \)’th eigenstate in either the left or right lead respectively. The other vectors \( d^\dagger \) and \( c \) contain creation operators for the system and the leads respectively and are obtained by taking the Hermitian conjugate of the vectors introduced in Eq. (4.1.5). This setup will also allow us to eventually
include energy filtered leads. The energy filtered leads can then be considered as being a part of the system Hamiltonian $H_S(t)$. However the energy filters themselves are not driven. The current through this setup is simply the change in particle number in any of the three subsystems. Here we choose to define the current operator as the current through the left lead. It is simply given by the expectation value of the time derivative of the particle number times the charge of the relevant particle:

$$J_L(t) = -e \langle \frac{dN_L(t)}{dt} \rangle,$$

(4.1.6)

where the number operator is defined as $N_L(t) = \sum_{\alpha \in L} c_{\alpha}^\dagger(t) c_{\alpha}(t)$, $-e$ denote the electron charge and the brackets $\langle \cdot \rangle$ indicate that the expectation value of $\cdot$ is taken. For an equilibrium system the expectation value is given as the thermodynamic average which is:

$$\langle \cdot \rangle = \text{Tr}(\rho_0 \cdot), \quad \rho_0 = \frac{e^{-\beta(H_L^L - \mu N_L)}}{Z},$$

(4.1.7)

where $\rho_0$ denotes the initial density matrix of the left lead, $Z = \text{Tr}(e^{-\beta(H_L^L - \mu N_L)})$ denotes the partition function, $\beta$ is the inverse temperature $\beta = \frac{1}{k_B}$ of the left lead, $\mu$ is the chemical potential of the left lead, $H_L^L$ is the Hamiltonian for the left lead defined in Eq. (4.1.3) and $N_L$ is the number operator for the left lead. The average in Eq. (4.1.7) is taken with respect to the Hamiltonian for the left lead only. This is because initially the leads and the system are completely decoupled from each other and the thermodynamic properties of the left lead are determined from $H_L^L$ alone. If we assume the leads are in equilibrium before a bias voltage is applied the current is determined from Eqs. (4.1.6) and (4.1.7). The derivative of the number operator is computed using the Heisenberg equation of motion in Appendix B.1 and the result is:

$$J_L(t) = i\frac{e}{\hbar} \sum_{\alpha \in L} \left( V_{\alpha,n} \langle c_{\alpha}^\dagger(t) d_{\alpha}(t) \rangle - V_{\alpha,n}^* \langle d_{\alpha}^\dagger(t) c_{\alpha}(t) \rangle \right) = \frac{2e}{\hbar} \sum_n \text{Re} \left( V_{\alpha,n} i \langle c_{\alpha}^\dagger(t) d_{\alpha}(t) \rangle \right).$$

(4.1.8)

Besides the matrix elements that describes the system lead coupling the current depends only on the quantity $i \langle c_{\alpha}^\dagger(t) d_{\alpha}(t) \rangle$. This object is a particular example of what is known as a Green’s function. Green’s functions are an indispensable tool in quantum many-body systems and they can be used to compute various quantities in addition to the current, such as local density of states (LDOS), particle density, distribution functions and various types of correlations functions [37]. Therefore to compute the desired quantities we must first understand how Green’s functions work in non-equilibrium settings.

### 4.2 Keldysh formalism and Green’s functions

We start by briefly summarizing how Green’s functions are defined for equilibrium many body systems [1]. In such systems we are typically interested in the expectation value of some measurable quantity represented by some operator $\mathcal{O}$. The expectation value in equilibrium is

$$\langle \mathcal{O} \rangle = \langle \rho_0 | \mathcal{O} \rangle,$$

(4.2.1)

where $\rho_0$ is the equilibrium density matrix. In the language of second quantization the operators $\mathcal{O}$ in many body systems are expressed in terms of creation and annihilation operators. Therefore being able to compute the expectation value of these operators with respect to some Hamiltonian is of huge interest. We now introduce the different types of Green’s functions that are needed in equilibrium and in non-equilibrium [37]. First we define the lesser Green’s function

$$g<(t, t') = i \langle c_{\alpha}(t') c_{\alpha}(t) \rangle,$$

(4.2.2)

At equal times this Green’s function is $i \langle N(t) \rangle$, where $N(t)$ is the number operator. Therefore this particular Green’s function contains information about the number of particles in the system. More generally the lesser Green’s function $g<(t, t')$ contains information about which states in the system that are occupied. In the same spirit we now define the greater Green’s function as

$$g>(t, t') = i \langle c_{\alpha}(t) c_{\alpha}^\dagger(t') \rangle.$$

(4.2.3)

The definitions of all Green’s functions given in this thesis are valid for fermions.
The only difference from the lesser Green's function is that the two operators \( c(t) \) and \( c^\dagger (t') \) are swapped. At equal times the greater Green's function is \( i(1 - N(t)) \) where \( N(t) \) is the number operator. In condensed matter physics the quantity \( (1 - N(t)) \) has a natural interpretation, since one may think of the absence of an electron as a hole. So the quantity can be thought of as number operator for holes. In addition to the lesser and greater Green's function we now define the retarded and the advanced Green's function

\[
g^{r/a}(t,t') = \mp i\theta(\pm t \mp t') \langle \{ c(t), c^\dagger (t') \} \rangle, \tag{4.2.4}
\]

where the brackets denote the anti-commutator, \( \theta \) is the Heaviside step function, the superscript \( r \) denotes the retarded Green's function and the superscript \( a \) denotes the advanced Green's function. These two Green's functions contain information on the spectra of many body systems. We now introduce the time-ordered Green's function

\[
g^T(t,t') = -i\langle T \{ c^\dagger (t'), c(t) \} \rangle = -i\theta(t'-t)\langle c^\dagger (t')c(t) \rangle + i\theta(t-t')\langle c(t)c^\dagger (t') \rangle, \tag{4.2.5}
\]

where \( T \) denotes the time ordering operator. This operator orders operators with earlier times to the right of those who are later. Analogously we define the anti-time ordered Green's function:

\[
g^{\bar{T}}(t,t') = -i\langle \bar{T} \{ c^\dagger (t'), c(t) \} \rangle = -i\theta(t'-t)\langle c^\dagger (t')c(t) \rangle + i\theta(t-t')\langle c(t)c^\dagger (t') \rangle, \tag{4.2.6}
\]

where \( \bar{T} \) denotes the anti time-ordering operator, which works like the time-ordering operator accept it puts later times to the right of those who are earlier. In the expressions defined above the time evolution is taken with respect to the full Hamiltonian of the system. We refer to this type of Green's function as the full Green's function. Sometimes the time evolution in a Green's function is not taken with respect to the full Hamiltonian. If for instance the time evolution is taken only with respect to a subsystem or the non-interacting part of a Hamiltonian, we instead refer to the Green's functions as the bare Green's functions. To distinguish the full Green's functions and the bare Green's functions, the ladder are given the subscript 0. In equilibrium many body systems all the Green's functions defined so far can be expressed in terms of the time-ordered Green's function. For this Green's function a perturbative theory can be developed \(^2\). This is rather technical and because we won't be applying the full machinery here it is not something we will go into detail with [38]. However we will simply make a mental note that it is possible, which will be important when we consider non-equilibrium settings.

![Figure 4.1: Picture of the Keldysh contour. The time \( \tau_1 \) is on the forward branch and the time \( \tau_2 \) is on the backward branch. This picture is found in [39].](image)

We now consider non-equilibrium systems. We will focus on systems which are initially in equilibrium at time \( t = t_0 \) and therefore have a well defined initial state \( \rho_0 \). The expectation value of some physical operator for times \( t > t_0 \) is then

\[
\langle O(t) \rangle = \text{Tr}(\rho_0 O(t)). \tag{4.2.7}
\]

Here however there is no guarantee that a quantum state returns to its initial state once the system has left equilibrium. As a result Green's functions generally don’t have symmetry between their two times \( g(t,t') \neq g(t-t') \). This is an important requirement for the equilibrium perturbative expansion to work. It turns out it is still possible to derive a structurally similar result for non-equilibrium systems. One way to do so is to introduce the so called *Keldysh contour*. The Keldysh contour is a contour in the complex plane where time is treated as a complex variable \( \tau \). Time then runs from some initial time \( t_0 \) to the time of interest \( t \) and then all the way back to \( t_0 \). This is depicted in Fig. 4.1. The contour has two branches. The first one is the forward branch where time runs from \( t_0 \) to \( t \). The second one is the backward branch where time runs from \( t \) back to \( t_0 \). The advantage of this approach is that expectation values can still be taken with respect to some initial density matrix \( \rho_0 \) if one assumes the system to start in equilibrium at \( t_0 \) [38]. For instance in the two terminal setup introduced in Eq. (4.1.1) the

\(^2\)At finite temperatures one often defines Matsubara Green's functions where time is imaginary and then perform analytic continuation back to real variables.
contacts are in equilibrium before a voltage bias is turned on. Typically one considers cases where the initial state is known in the far past \( t_0 = -\infty \). This is equivalent to ignoring the transient regime which is the period of time right after the system leaves equilibrium before relaxation processes brings it into a steady state (if the system has one that is). While this approach ignores the transient regime it is very useful to find the steady state configuration that the system assumes after sufficiently long time has passed. Furthermore the notion of time-ordering from equilibrium has to be extended such that times are ordered according to their position on the contour. In analogy with time-ordering one therefore defines contour-ordering as putting operators with times earlier on the contour to the right of operators with times later on the contour. In analogy with the time-ordered Green’s function we therefore define the contour ordered Green’s function as

\[
g^c(\tau, \tau') = -i \langle \mathcal{T}_C \{ c(\tau'), c(\tau) \} \rangle, \quad g^c(\tau, \tau') = \begin{cases} g^T(\tau, \tau') & \text{if } \tau, \tau' \in \mathcal{C}_1 \\ g^\gamma(\tau, \tau') & \text{if } \tau \in \mathcal{C}_1, \tau' \in \mathcal{C}_2 \\ g^\epsilon(\tau, \tau') & \text{if } \tau \in \mathcal{C}_2, \tau' \in \mathcal{C}_1 \\ g^\tau(\tau, \tau') & \text{if } \tau, \tau' \in \mathcal{C}_2 \end{cases}, \tag{4.2.8}
\]

where \( \mathcal{T}_C \) denotes the contour-ordering operator, \( \mathcal{C}_1 \) denotes to forward branch and \( \mathcal{C}_2 \) denotes the backward branch. A more useful way to write the contour-ordered Green’s function is to introduce a Keldysh space. The contour-ordered Green’s function is then a 2x2 matrix which contains the four different options in Eq. (4.2.8). The contour ordered Green’s function may then be written as:

\[
g^c(\tau, \tau') = \begin{bmatrix} g^T(\tau, \tau') & g^\epsilon(\tau, \tau') \\ g^\gamma(\tau, \tau') & g^\tau(\tau, \tau') \end{bmatrix}. \tag{4.2.9}
\]

Just as the time-ordered Green’s function can be used to construct a perturbative expansion in equilibrium at zero temperature, the contour ordered Green’s function can be used to construct the a non-equilibrium perturbative expansion. Here knowing the initial state of the system at \( t_0 \) is the key. The price one has to pay is that time now lives on the Keldysh contour and that the symmetry between two different times are broken. However the expansion is structurally similar to the equilibrium case except for the fact that the times \((t, t')\) should be replace by the contour times \((\tau, \tau')\) and that contour-ordering replaces time-ordering [38, 39]. We will exploit this structural equivalence later for computations. Because the contour ordered Green’s function has a matrix structure any product between contour ordered objects has an additional \( 2 \times 2 \) matrix structure. If we consider an equation of motion for the contour ordered Green’s function in terms of other contour ordered objects it is not trivial how the different matrix entries in Eq. (4.2.9) will depend on these quantities. To get an expression we have to perform analytic continuation. To do this we will apply the so called Langreth technique. One can derive several Langreth identities, by using this method but it becomes rather lengthy and once the basic idea is in place not something which is difficult to do. Since we will only be using this technique for technical computations it can be found among the other appendices for this chapter. In Appendix (B.2) the Langreth procedure is illustrated by performing analytic continuation on the lesser component of a contour ordered object. Besides serving as an instructive example this result will be important for computations later in the thesis.

The four different Green’s functions in the matrix in Eq. (4.2.9) are not linearly independent. One can relate the retarded- and advanced Green’s functions to the lesser-, greater-, time-ordered- and anti time-ordered Green’s functions through the following identities:

\[
g^r(t, t') = g^1(t, t') - g^\epsilon(t, t') = g^\gamma(t, t') - g^\tau(t, t'). \tag{4.2.10}
\]

\[
g^a(t, t') = g^1(t, t') - g^\gamma(t, t') = g^\epsilon(t, t') - g^\tau(t, t'). \tag{4.2.11}
\]

Therefore it is sometimes useful to get rid of this redundancy by defining the Keldysh Green’s function as

\[
g^k(t, t') \equiv g^\gamma(t, t') + g^\epsilon(t, t') = g^1(t, t') + g^\tau(t, t'). \tag{4.2.12}
\]

Together with the retarded- and advanced Green’s function the Keldysh function can be used to define a new basis where only 3 Greens functions are needed. A particular useful basis is the Larkin-Ovchinnikov basis [40]. In this basis one defines a new contour Green’s function through the transformation

\[
g_c^c = L \tau^3 g_c L^\dagger, \quad L = \frac{1}{\sqrt{2}}(\tau^0 - i\tau^2), \tag{4.2.13}
\]

\[27\]
where $\tau^i, i = 1, 2, 3$ denotes the Pauli matrices and $\tau^0$ is the $2 \times 2$ identity matrix. In the new basis the contour Green’s function becomes

$$\mathbf{g}^c = \begin{bmatrix} g^R & g^K \\ 0 & g^A \end{bmatrix}$$  (4.2.14)

This basis is very useful since it makes some practical computations more simple.

During calculations we will encounter products of matrices, both those defined in Keldysh space as well as matrices with a physical space. To tell different products apart we will be using the following notation

1. We will encounter terms of the form $AB$ which simply means the matrix product of $A(t, t')$ and $B(t, t')$.

2. We will encounter products of the form $A \circ B$ which means matrix product and convolution in time:

$$A \circ B = \int_{-\infty}^{\infty} dt_1 A(t, t_1) B(t_1, t').$$  (4.2.15)

3. We will encounter products of the form $A \otimes B$. Where $\otimes$ denotes the Keldysh product. This product is to be understood in the following sense:

$$A \otimes B = \int_{-\infty}^{\infty} dt_1 A(t, t_1) \otimes B(t_1, t').$$  (4.2.16)

$$= \int_{-\infty}^{\infty} dt_1 \begin{bmatrix} A(t, t_1)_{11} & A(t, t_1)_{12} \\ A(t, t_1)_{21} & A(t, t_1)_{22} \end{bmatrix} \begin{bmatrix} B(t_1, t')_{11} & B(t_1, t')_{12} \\ B(t_1, t')_{21} & B(t_1, t')_{22} \end{bmatrix}.$$  (4.2.17)

This last type of product only becomes necessary when the matrices are defined on the Keldysh contour such as if we are dealing with the time-ordered Green’s function.

For computations in this thesis we will be using Green’s functions with different species of fermionic operators. To distinguish Green’s functions that describe different parts of the setup we will be using the following notation. $G$ denotes a Greens function involving only system operators $d, d^\dagger$. $\mathcal{G}$ denotes a Green’s function which contains one system operator $d$ and one lead operator $c$. $g$ denotes a Green’s function describing the leads and therefore only contain the lead operators $c^\dagger, c$.

### 4.2.1 Green’s functions in driven systems

In non-equilibrium systems the symmetry between the times $t$ and $t'$ in the Green’s functions of the system is broken. That means we can not generally claim $G(t, t') \neq G(t', t)$ for any type of Green’s function. This is an issue we have to address since we would like to obtain the Green’s functions in the energy domain. This is normally done via a Fourier transform in the time difference $t - t'$ [37]. Due to the time periodicity of the Hamiltonian the Green’s functions do however contain discrete time translational symmetry, which we will now exploit. The following considerations can be done for any type of Green’s function for a periodically driven system, but for concreteness we focus on the retarded Green’s function. There are two time scales in the problem. One associated with the dynamics of the system over long time scales and one with the dynamics over one period in time. It is therefore useful to define the Fourier transform of the retarded Green’s function as:

$$G^r(t, \mathcal{E}) = \int_{-\infty}^{\infty} dt' G^r(t, t') e^{-i\mathcal{E}(t'-t)} = \int_{-\infty}^{\infty} ds G^r(t, t-s) e^{i\mathcal{E}s},$$  (4.2.18)

Where $s = t - t'$. The corresponding inverse Fourier transform is then

$$G^r(t, t-s) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\mathcal{E} G^r(t, \mathcal{E}) e^{-i\mathcal{E}s}.$$  (4.2.19)

The function $G^r(t, \mathcal{E})$ still has discrete time translational symmetry in the remaining time variable. Therefore it has a Fourier decomposition:

$$G^r(t, \mathcal{E}) = \sum_{n=-\infty}^{\infty} e^{-i\mathcal{E}n} G^{r(n)}(\mathcal{E}),$$  (4.2.20)
where the Fourier components $G^{r(n)}(\epsilon)$ are what we refer to as \textit{retarded Floquet Green’s functions}, \( n \) is an integer and $\Omega = \frac{2\pi}{T}$ is the driving frequency with period $T$. The Fourier components are given by

$$G^{r(n)}(\epsilon) = \frac{1}{T} \int_{0}^{T} dt e^{i n \Omega t} G^r(t, \epsilon). \quad (4.2.21)$$

The choice of transform in Eq. (4.2.18) is not unique. Sometimes it is favorable to work with different transforms of the energy. For the applications in this thesis this choice won’t make a difference.

Now that we now how to deal with Green’s functions for periodically driven systems we are ready to find an equation of motion for the retarded Green’s function that describes the periodically driven system in Eq. (4.1.2). Since we are considering non-interacting systems we can actually obtain a closed expression for $G^r(t, t')$. This is done in Appendix B.3 were the the following equation is obtained:

$$\left( i \frac{d}{dt} + \epsilon - H_S(t) \right) G^r(t, \epsilon) - \int_{-\infty}^{\infty} dt \Sigma^r(\tau) G(t - \tau, \epsilon) = 0, \quad (4.2.22)$$

where $\Sigma^r(\tau) = V^\dagger g_0^\dagger(\tau) V$ is the retarded self energy arising from the fact that the system is coupled to two external leads. Here $g_0^\dagger(\tau)$ denotes the bare Green’s function for the leads and the couplings $V$ and $V^\dagger$ are the coupling matrices introduced in Eq. (4.1.4). The self energy depends on the specific choice of contact and generally the self energy will be some functional $\Sigma^r(\epsilon)$. It is not generally possible to obtain an analytic expression for this self energy so approximations are needed. One option is to treat the problem perturbatively in the coupling [9]. Another very non-restrictive obtain is to consider the so called \textit{wide-band limit} [39]. This is an approximation for the self energy, that has two assumptions built in. The first one is that we assume the real part of the self energy $\Sigma^r(\epsilon)$ to be zero. Even if this is in fact not true and there might some real part this will simply be a correction to the energy $\epsilon$ in the system Green’s function $G^r(\epsilon)$ which will not change our results qualitatively. The second assumption of the approximation is that one assumes that the imaginary part $-i \Gamma$ of the retarded self energy is independent of energy. To understand what this entails we will first look at the self energy in the energy domain. By a Fourier transform one finds that

$$\Sigma^r(\epsilon) = V^\dagger g_0^\dagger(\epsilon) V. \quad (4.2.23)$$

The coupling matrices contain the components $V_{\alpha,m}$ where the index $\alpha$ denotes lead eigenstates and the index $m$ denotes system eigenstate in the site basis. Typically the leads large enough that one may instead write the elements as smooth function of the lead energies: $V_m(\epsilon_\alpha)$. The imaginary part $-i \Gamma(\epsilon)$ of this self energy is given by

$$-\text{Im} (\Sigma^r(\epsilon)) = -\frac{\left( V^\dagger(\epsilon_\alpha) g_0^\dagger(\epsilon) V(\epsilon_\alpha) - V^\dagger(\epsilon_\alpha) g_0^\dagger(\epsilon) V(\epsilon_\alpha) \right)}{2}$$

$$= -\text{Im}(V^\dagger(\epsilon) \left( g_0^\dagger(\epsilon) - \frac{(g_0^\dagger(\epsilon))^\dagger}{2} \right) V(\epsilon)) = V^\dagger(\epsilon_\alpha) \frac{-\text{Im}(g_0^\dagger(\epsilon))}{2} V(\epsilon_\alpha)$$

$$V^\dagger(\epsilon_\alpha) \left( \pi \sum_{\alpha \in L,R} \delta(\epsilon - \epsilon_\alpha) \right) V(\epsilon_\alpha) = \frac{2\pi}{2} \left( V^\dagger(\epsilon) \rho_L(\epsilon) V(\epsilon) + V^\dagger(\epsilon) \rho_R(\epsilon) V(\epsilon) \right)$$

$$= \frac{\Gamma_L(\epsilon) + \Gamma_R(\epsilon)}{2}, \quad (4.2.24)$$

where we defined the density of states for the $\alpha$’th lead $\rho_\alpha(\epsilon) = \sum_{\alpha \in L,R} \delta(\epsilon - \epsilon_\alpha)$ and the transition rate matrices $\Gamma_L/R(\epsilon) = 2\pi V^\dagger(\epsilon) \rho_L(\epsilon) V(\epsilon)$. From this expression we see that the transition rate matrices $\Gamma_L/R(\epsilon)$ obey an equation similar to that given by Fermi’s golden rule. This is actually quite surprising since our result is not perturbative while Fermi’s golden rule is a standard result within first order time-dependent perturbation theory. The assumption that the imaginary part is independent of energy implies that we assume that the density of states for both leads is independent for energy, and also that the system-lead coupling is independent of energy. That is we assume that each state of the system is coupled to all states in the lead with the same coupling strength. These assumptions are generally expected to work well as long as the bandwidth of the leads are large. In the wide-band limit the self energy is then $\Sigma^r(\epsilon) = -i \Gamma = -\frac{\Gamma_L + \Gamma_R}{2}$. In the time domain this is equivalent to: $\Sigma^r(t, t') = -i \delta(t - t')$. In light of
this observation the wide-band limit has an alternative interpretation in the time domain. In the time
domain the delta function essentially picks out the part of the function \( G^r(t−τ, \mathcal{E}) \) where \( τ = 0 \). That is
in the time domain the wide-band limit is equivalent to assuming the system has no memory of its state
at any previous time due to the delta function. This is also sometimes called a Markov approximation.
By applying the wide-band limit to the equation of motion for \( G^r(t, \mathcal{E}) \) we get the equation
\[
\left( \mathcal{E} + i\frac{d}{dt} - \hat{H}_S(t) \right) G^r(t, \mathcal{E}) = 1.
\]
where we defined:
\[
\hat{H}_S(t) = H_S(t) - i\Gamma.
\]
In order to compute physical properties we will need the retarded Floquet Green’s functions \( G^{r(n)}(\mathcal{E}) \).
They can be obtained through the Green’s functions \( G^r(t, \mathcal{E}) \). Therefore we start from the equation of
motion in Eq. (4.2.25). We start by taking multiplying both sides of the equation with \( \exp(in\Omega t) \) and
taking the time average to get:
\[
\frac{1}{T} \int_0^T e^{in\Omega t} (\mathcal{E} + i\frac{d}{dt}) G^r(t, \mathcal{E}) - \frac{1}{T} \int_0^T e^{in\Omega t} \hat{H}_S(t) G^r(t, \mathcal{E}) = \delta_{n,0} I
\]
\[
⇔ (\mathcal{E} + n\Omega) G^{r(n)}(\mathcal{E}) - \frac{1}{T} \int_0^T e^{in\Omega t} \hat{H}_S(t) G^r(t, \mathcal{E}) = \delta_{n,0} I.
\]
Now we write the retarded Floquet Green’s function and the Hamiltonian in terms of their Fourier
components:
\[
\hat{H}_S(t) = \sum_{m=-\infty}^{\infty} e^{-im\Omega t} \hat{H}^{(m)}_S,
\]
\[
G^r(t, \mathcal{E}) = \sum_{k=-\infty}^{\infty} e^{-ik\Omega t} G^{r(k)}(\mathcal{E}).
\]
The expression in Eq. (4.2.27) can then be written as:
\[
(\mathcal{E} + n\Omega) G^{r(n)}(\mathcal{E}) - \sum_{m,k=-\infty}^{\infty} \left( \frac{1}{T} \int_0^T dt e^{i(n-k-m)\Omega t} \right) \hat{H}^{(m)}_S G^{r(k)}(\mathcal{E}) = \delta_{n,0} I,
\]
which becomes:
\[
(\mathcal{E} + n\Omega) G^{r(n)}(\mathcal{E}) - \sum_{k=-\infty}^{\infty} \hat{H}^{(n-k)}_S G^{r(k)}(\mathcal{E}) = \delta_{n,0} I.
\]
This can be written as a matrix equation what was done for the Floquet sidebands within the extended
space formalism introduced in section 2.2:
\[
\left( \begin{array}{c}
\mathcal{E} + \Omega \\
\mathcal{E} \\
\mathcal{E} - \Omega \\
\end{array} \right)
\left( \begin{array}{c}
\mathcal{E} + \Omega \\
\mathcal{E} \\
\mathcal{E} - \Omega \\
\end{array} \right)
\left( \begin{array}{c}
\cdots \\
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\hat{H}^{(-1)} \\
\cdots \\
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\hat{H}^{(-1)} \\
\cdots \\
\hat{H}^{(0)} \\
\hat{H}^{(-1)} \\
\cdots \\
\hat{H}^{(1)} \\
\hat{H}^{(-1)} \\
\cdots \\
\hat{H}^{(0)} \\
\hat{H}^{(-1)} \\
\cdots \\
\hat{H}^{(1)} \\
\hat{H}^{(-1)} \\
\cdots \\
\hat{H}^{(0)} \\
\hat{H}^{(-1)} \\
\cdots \\
\hat{H}^{(1)} \\
\hat{H}^{(-1)} \\
\cdots \\
\hat{H}^{(0)} \\
\hat{H}^{(-1)} \\
\cdots \\
\hat{H}^{(1)} \\
\end{array} \right)
\left( \begin{array}{c}
G^{r(1)}(\mathcal{E}) \\
G^{r(0)}(\mathcal{E}) \\
G^{r(-1)}(\mathcal{E}) \\
\vdots \\
\vdots \\
\end{array} \right) = \left( \begin{array}{c}
\vdots \\
\vdots \\
\vdots \\
\vdots \\
\vdots \\
\end{array} \right).
\]
While this method for finding retarded Floquet Green’s functions is well suited for numerical applications
it is not very physically illuminating. It is possible to analytically different representation for the retarded
Floquet Green’s functions, that allow us to give an physical interpretation of these quantities. To do so
it is useful to expand the retarded Floquet Green’s functions in terms of Floquet states. This is done in
Appendix B.4 where we obtain:
\[
G^{r(n)}(\mathcal{E}) = \sum_{m=-\infty}^{\infty} \sum_{\alpha} |\phi_{\alpha}^{-(m-n)}(\mathcal{E})\rangle \langle \phi_{\alpha}^{+(m)}(\mathcal{E})|_{\mathcal{E} - (\epsilon_{\alpha} - i\gamma_{\alpha})}
\]
where \( \epsilon_{\alpha} \) is the quasienergy of the Floquet state \( |\phi_{\alpha}\rangle \) and \( -i\gamma_{\alpha} \) is the imaginary part of that quasienergy
due to the coupling to external leads. The \( \pm \) signs on the ket indicate whether it is a left or right
eigenstate. Due to the non-Hermicity of $\hat{H}_S(t)$ a bi-orthonormal basis is needed to form a complete basis set \cite{14}. A physical interpretation of the numerator is that it transfers a Floquet sideband in the $m$ photon subspace into the $m-n$ photon subspace by absorbing ($n>0$) or emitting ($n<0$) $n$ photons. Since all the harmonics have different weight the different photon sectors are not on equal footing. We now unfold the Floquet Brillouin zone by writing the quasienergy as $\epsilon$. Since all the harmonics have different weight the different photon sectors are not on equal footing. We now unfold the Floquet Brillouin zone by writing the quasienergy as $\epsilon = E_\alpha + m\Omega$. We may then write Eq. (4.2.32) as

$$G^{r(n)}(\mathcal{E}) = \sum_{m=-\infty}^{\infty} \sum_\alpha \frac{|\phi^{-(m-n)}_\alpha\rangle \langle \phi^{+(m)}_\alpha|}{\mathcal{E} - E_\alpha - m\Omega + i\gamma_\alpha}.$$  \hspace{1cm} (4.2.33)

The advantage of this representation is that the Green’s function at a specific energy depends on an actual energy eigenstate $E_\alpha$ of the periodically driven system. This representation is more natural to work with since the external leads are non-driven and therefore the notion of quasienergy does not apply to them. Therefore it is more natural to have an unfolded spectrum such that everything is expressed in energy. This is exactly what the equation above allow us to do. For numerical computations Eq. (4.2.32) is truncated such that it contains a finite number of copies. The physical interpretation of Eq. (4.2.33) given above, implies that in order to capture processes that involves the absorption or emission of several photons more copies has to be kept in order to get the correct result. Now that we know how to work with Green’s functions in driven systems we can return to the original problem stated namely finding the current through the setup defined in Eq. (4.1.1).

### 4.3 Time-averaged current and differential conductance

#### 4.3.1 General expression for the current

Now that a useful framework to describe the non-equilibrium setting introduced in section 4.1 has been established we turn our attention to the expression for the current in Eq. (4.1.8). By inspection we see that it can be expressed in terms of an equal time non-equilibrium lesser Green’s function

$$J_L(t) = \frac{i\hbar}{\epsilon_a} \sum_{n} V_{a,n} c_n^<(t) d_n(t) - V_{a,n}^* d_n^<(t) c_n(t) = \frac{2e}{\hbar} \sum_{n} \text{Re} \left( V_{a,n} G_{a,n}(t,t) \right).$$  \hspace{1cm} (4.3.1)

In Appendix B.5 the lesser Green’s function $G_{a,n}(t,t')$ is found:

$$G_{a,n}^<(t,t') = \int_{-\infty}^{\infty} dt_1 \sum_m V_{a,m}^* (G_{nm}^r(t_1,t_1) g_{a,n}^<(t_1,t') + G_{nm}^< (t_1,t) g_{a}^a(t_1,t')).$$  \hspace{1cm} (4.3.2)

We now put $t = t'$ in Eq. (4.3.2) and plug it into the expression for current in Eq. (4.3.1) to get:

$$J_L(t) = \frac{2e}{\hbar} \text{Re} \left[ \sum_{n} V_{a,n} \int_{-\infty}^{\infty} dt_1 V_{a,m}^* (G_{nm}^r(t_1,t_1) g_{a,n}^<(t_1,t) + G_{nm}^< (t_1,t) g_{a}^a(t_1,t)) \right].$$  \hspace{1cm} (4.3.3)

The two bare lead Green’s functions $g_{0a}^<(t_1,t)$ and $g_{0a}^a(t_1,t)$ are given by

$$g_{0a}^<(t-t') = i e^{i\epsilon_a (t-t')} \langle c_0^<(t) c_0^a(0) \rangle = i e^{i\epsilon_a (t-t')} f(\epsilon_a).$$  \hspace{1cm} (4.3.4)

$$g_{0a}^a(t-t') = \mp i \theta(\pm t \mp t') e^{-i\epsilon_a (t-t')} \langle \{ c_0^a(0) c_0(0) \} \rangle = \mp i \theta(\pm t \mp t') e^{-i\epsilon_a (t-t')}. $$  \hspace{1cm} (4.3.5)

The current in Eq. (4.3.3) can then be written as:

$$J_L(t) = \frac{2e}{\hbar} \text{Re} \left[ \sum_{n} \int_{-\infty}^{\infty} dt_1 V_{a,n} V_{a,m}^* e^{-i\epsilon_a (t_1-t)} (G_{nm}^r(t_1,t_1) f(t_1) + G_{nm}^< (t_1,t_1) \theta(t-t_1)) \right].$$  \hspace{1cm} (4.3.6)

Now we use that $\text{Re}(iz) = -\text{Im}(z)$, where $z$ is some complex number. We can then write Eq. (4.3.6) as:

$$J_L(t) = -\frac{2e}{\hbar} \text{Im} \left[ \sum_{n} \int_{-\infty}^{\infty} dt_1 V_{a,n} V_{a,m}^* e^{-i\epsilon_a (t_1-t)} (G_{nm}^r(t_1,t_1) f(t_1) + G_{nm}^< (t_1,t_1) \theta(t-t_1)) \right].$$  \hspace{1cm} (4.3.7)
We now assume that the couplings $V_{\alpha,n}V_{\alpha,m}^*$ are smoothly varying functions of energy. That is we assume that we may write $V_{\alpha,n} = V_{\alpha}(\epsilon_\alpha)$. We can then insert an integral over energy with a delta function into Eq. (4.3.7) to obtain:

$$J_L(t) = -\frac{2e}{\hbar} \text{Im} \left[ \sum_{m,n} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dE \delta(E - \epsilon_\alpha) V_n(\epsilon_\alpha) V_m^*(\epsilon_\alpha) e^{-i\epsilon_\alpha(t_1 - t)} \times \left( G_{nm}^<(t,t_1) f_L(\epsilon_\alpha) + G_{nm}^<(t,t_1) \theta(t - t_1) \right) \right].$$

(4.3.8)

Using the delta function we can exchange $\epsilon_\alpha$ everywhere in Eq. (4.3.8) with $E$ and rearrange terms to get:

$$J_L(t) = -\frac{2e}{\hbar} \text{Im} \left[ \sum_{m,n} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dE V_m^*(E) \left( \sum_{\alpha \in L} \delta(E - \epsilon_\alpha) \right) V_n(E) e^{-iE(t_1 - t)} \times \left( G_{nm}^<(t,t_1) f_L(E) + G_{nm}^<(t,t_1) \theta(t - t_1) \right) \right].$$

(4.3.9)

The sum over delta functions is the total density of states in the left lead: $\rho_L(E) = \sum_{\alpha \in L} \delta(E - \epsilon_\alpha)$. We now define the transition rate matrix:

$$\Gamma_{Lmn}(E) = 2\pi(V_{L,m}(E))^* \rho_L(E) V_{L,n}(E).$$

(4.3.10)

We now contract indices in Eq. (4.3.9), use that $2\pi\hbar = h$ and apply the expression for the transition rate matrix to write the equation for the current as

$$J_L(t) = -\frac{2e}{\hbar} \int_{-\infty}^{\infty} dE \int_{-\infty}^{\infty} dt_1 \text{Im} \left[ e^{-iE(t_1 - t)} \text{Tr} \left( \Gamma_L(E) \left( G^r(t,t_1) f_L(E) + G^<(t,t_1) \theta(t - t_1) \right) \right) \right].$$

(4.3.11)

This is a famous result first obtained by Jauho Wingreen and Meir [39]. Although we won’t be considering the effects of interactions it is worth noticing that the expression for the current in Eq. (4.3.11) is quite general. As long as the leads stay non-interacting the result even extends to interacting systems although we left out expressions with four or more operators in Eq. (4.1.2). This is essentially because the contribution to the current in Eq. (4.1.8) arises from the tunneling term alone. It is however difficult to obtain general expressions for Green’s functions in the interacting case. The model which was introduced in Eq. (4.1.1) to derive the current, is slightly different from the one used in the paper by Jauho Wingreen and Meir [39]. In the paper there is additional time dependence in the tunneling Hamiltonian as well as the Hamiltonian for the contacts. In the paper they consider the possibility that the coupling between leads and system $V_{\alpha,m}$ can depend on time. One way to achieve this is to make a setup like the one described above, but with quantum point contacts included in the setup. It is then possible to tune the coupling between the system and leads by changing the external voltage on the quantum point contacts over time. However for simplicity we will consider coupling matrices that are constant in time. Furthermore the paper assumes that the energies $\epsilon_\alpha$ in the leads can be time-dependent by replacing $\epsilon_\alpha$ with $\epsilon_\alpha(t) = \epsilon_\alpha^0 + \Delta_\alpha(t)$. This becomes relevant if an AC-bias is introduced into the transport setup. For the systems considered here this won’t be the case therefore this time dependence is neglected as well. Although we neglect some of the time-dependence included in the original paper, the method used to obtain the more general result is same as to one used here.

### 4.3.2 Time-averaged current through a periodically driven non-interacting system

Our goal is to describe transport through non-interacting periodically driven topological insulators. In the absence of interactions a more simple form for the current through such systems can be derived from the Jauho-Wingreen-Meir result. However due to the presence of the external drive the current at any given moment in time does necessarily display any significant features. Rather we focus on the time averaged current:

$$\langle J_L(t) \rangle = \frac{1}{T} \int_0^T dt J_L(t).$$

(4.12)
Appendix B.7 for a full derivation. The time averaged current is given by technical computation. Here we will simply state the result while the interested reader may consult Appendix B.7 for a full derivation. The time averaged current is given by

\[
\langle J_L(t) \rangle = \frac{e}{h} \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} d\epsilon \left( T_{RL}^{(n)}(\epsilon) f_L(\epsilon) - T_{LR}^{(n)}(\epsilon) f_R(\epsilon) \right),
\]

where the functions \( f_{L/R}(\epsilon) \) are Fermi-Dirac distributions for left and right lead respectively.\(^3\) The quantities \( T_{\alpha\alpha}^{(n)}(\epsilon) \) are transmission probabilities given by:

\[
T_{\alpha\alpha}^{(n)}(\epsilon) \equiv \text{Tr} \left[ \left( G^{(n)}(\epsilon) \right)^{\dagger} \Gamma_{\alpha}(\epsilon + n\Omega) G^{(n)}(\epsilon) \Gamma_{\alpha}(\epsilon) \right].
\]

The formula for the current in Eq. (4.3.14) bears a close resemblance to the Landauer-Büttiker formula for non-driven non-interacting systems. The only difference is the harmonic index \( n \) which is also present in the retarded Floquet Green’s functions. The transmission formula can be interpreted as follows. The matrix \( \Gamma_{\alpha} \) is a matrix that describes how system and lead are coupled at energy \( \epsilon \). It describes the rate at which particles dissipate into or out of the system. The Green’s functions describe the propagation of particles once inside the system. Both the Green’s function and its hermitian conjugate are present since probabilities usually involve the modulus squared of the relevant quantity. So the formula may be interpreted as the probability of a particle entering with energy \( \epsilon \) from the lead \( \alpha' \) then propagating around the system at energy \( \epsilon \) while absorbing \( n > 0 \) or emitting \( n < 0 \) \( n \) photons from the drive and then exiting into the \( \alpha \)’th lead, described by \( \Gamma_{\alpha}(\epsilon + n\Omega) \), at the new energy \( \epsilon + n\Omega \). The total current is then obtained by summing up the different transmission probabilities and integrating this sum over energy weight by the distribution functions of the two leads. To derive the formula above we didn’t make any assumptions about the initial occupation inside the mesoscopic region. In fact the steady state is determined from the initial distribution functions in the leads \( f_{L}(\epsilon) \) and \( f_{R}(\epsilon) \) alone. This is due to the fact that we neglected interactions. More generally the current will some non-linear function of the occupation inside the system.

A crucial difference between the result for the current found here and the normal Landauer-Büttiker result is that the current does not necessarily vanish at zero bias. In periodically driven systems so called pumping currents are possible and for this reason one has to carefully choose the periodically driven material as well as the geometry of contacts. For a two-terminal setup, having inversion symmetry is enough to rule out a pumping current [25]. This result is rather intuitive since flipping the system upside down makes it look the same. Therefore there is no difference between going left or right at zero bias and therefore a current has to be absent. However in multiterminal systems this is not enough. It is also possible to derive a Floquet-Landauer-Büttiker formula for such a setup. The analysis is similar to what we have done here. Instead one should define the current through an arbitrary terminal \( \alpha \) [9, 25]. The formula looks similar but instead becomes

\[
\langle J_\alpha(t) \rangle = \frac{e}{h} \sum_{\beta \neq \alpha} \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} d\epsilon \left( T_{\beta\alpha}^{(n)}(\epsilon) f_{\alpha}(\epsilon) - T_{\alpha\beta}^{(n)}(\epsilon) f_{\beta}(\epsilon) \right),
\]

where the sum \( \beta \) is over all the different terminals accept for the \( \alpha \)'th one. In a multiterminal configuration the geometry has to be picked carefully to rule out any pumping current and in actual experiments a small contact asymmetry is enough to allow a pumping current to flow. In this thesis we wont be studying pumping currents or multiterminal configurations, but we have to keep in mind that they exist in more general circumstances. We now consider the two-terminal configuration. Instead of directly computing

\(^3\)This result is not new and have been obtained by many other people. For instance it may be found in the papers [9, 14, 25].
the current we will instead compute the differential conductance. That is the conductance to linear order
in applied bias voltage. Before we do so, we will first define the quantities
\[
\Delta f(E) = f_L(E) - f_R(E),
\]
\[
\bar{f}(E) = \frac{1}{2} (f_L(E) + f_R(E)),
\]
\[
\Delta T^n(E) = T_{LR}^{(n)}(E) - T_{RL}^{(n)}(E),
\]
\[
\bar{T}^n(E) = \frac{1}{2} \left( T_{LR}^{(n)}(E) + T_{RL}^{(n)}(E) \right).
\]

The current in Eq. (4.3.14) can then be written as
\[
\langle J_L(t) \rangle = \frac{e}{\hbar} \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} dE \left( \bar{T}^n(E) \Delta f(E) - \Delta T^n(E) \bar{f}(E) \right).
\]

In this form the current has two terms. One which is proportional to the bias difference like the one
present in non-driven systems and one which represents the contribution from the pumping current. We
now assume that the Fermi-Dirac distributions \( f_L \) and \( f_R \) have chemical potential \( \mu_L \) and \( \mu_R \) respectively
and that they are at the same temperature. Suppose that the chemical potential of the two leads are
separated by the bias voltage \( eV = \mu_1 - \mu_2 \). If the sign on the voltage is flipped it becomes \( eV = \mu_1 - \mu_2 \).
This is equivalent to exchanging \( \mu_1 \) and \( \mu_2 \). The function \( \bar{f}(E) \) is not affected by this interchange since
it is just the sum of the two distribution functions who only differ in chemical potential. In other words
\( \bar{f}(E) \) is an even function of the voltage difference \( eV \). Therefore the pumping current doesn’t have any
term linear in voltage. Therefore we need only consider the term \( \bar{T}^n(E) \Delta f(E) \). At small bias the current
is
\[
\langle J_L(t) \rangle = \frac{e^2}{\hbar} \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} dE \bar{T}^n(E) \left( -\frac{df_L(E)}{dE} \right) \varepsilon = \mu \times V.
\]

At zero temperature the derivative with a minus in front is just a delta function. In this temperature
limit the time-averaged differential conductance is therefore given by:
\[
\frac{d\langle J_L(t) \rangle}{dV}(\mu) = \frac{e^2}{\hbar} \sum_{n=-\infty}^{\infty} \frac{1}{2} \left( T_{RL}^{(n)}(\mu) + T_{LR}^{(n)}(\mu) \right).
\]

We introduced the wide-band limit in the equation of motion for the retarded Floquet Green’s function
and it should of course also be applied to physical quantities obtained via these Green’s functions.
Therefore the matrices transmission probabilities become
\[
T_{\alpha\alpha'}^{(n)}(E) = \text{Tr} \left[ (G_{\alpha\alpha'}^{(n)}(E))^\dagger \Gamma_\alpha G_{\alpha\alpha'}^{(n)}(E) \Gamma_{\alpha'} \right].
\]

### 4.4 Additional physical quantities obtained from Green’s functions

In addition to the differential conductance, Green’s functions can also be used to obtain several other
relevant quantities. First we will find a Floquet analog of the local density of states that is usually
obtained for non-driven systems. We will then find the time-averaged particle- and current density of
the steady state. Finally we will discuss how obtain non-equilibrium distribution functions for Floquet
topological insulators.

#### 4.4.1 Time-averaged density of states

The time averaged differential conductance only reveals whether or not the system transmits electrons
at a given energy. However it does not provide any information regarding the spectrum. While the
bandstructure, which is typically used to obtain the spectra of models, provide a nice insight for isolated
systems it doesn’t work for finite sized systems. Furthermore we saw that transport properties are
determined by the retarded Floquet Green’s function and that it is the Floquet sidebands \( |\phi_0^c\rangle \) that
mediate the transport. These states do not carry equal weight and quantifying this is an important step
in understanding transport signatures of periodically driven systems. We start by reviewing what is done for non-driven systems. For non-driven finite systems the density of states is usually what is calculated to obtain information on the spectra of many-body systems. The local density of states (LDOS) for non-driven systems is defined as

$$\rho_i(\mathcal{E}) = -\frac{\text{Im} \left( G_{r,i,i}(\mathcal{E}) \right)}{\pi}.$$ (4.4.1)

where the index $i$ refers to the site basis. Typically in many body systems one also defines the spectral function

$$A_\nu(\mathcal{E}) = -\frac{\text{Im} \left( G_{r,\nu,\nu}(\mathcal{E}) \right)}{\pi},$$ (4.4.2)

where $\nu$ is an eigenstate index. If the systems considered are translationally invariant the Green’s functions will be functions of crystal momentum. In that case the terminology spectral function is more common [37]. Since we are not however dealing with a system in equilibrium it is not so clear cut how to obtain something analogous from the two time Green’s function. Here one instead defines the time-averaged local density of states [27]:

$$\rho_i(\mathcal{E}) = -\frac{\text{Im} \left( G_{r,i,i}(0) \right)}{\pi},$$ (4.4.3)

and the time-averaged spectral function

$$A_0^\nu(\mathcal{E}) = -\frac{\text{Im} \left( G_{r,\nu,\nu}(0) \right)}{\pi}.$$ (4.4.4)

The reason for these definitions can be understood in terms of the expression for the retarded Floquet Green’s function in Eq. (4.2.33). If we for simplicity consider a non-interacting system without dissipative processes such that the finite imaginary part $i\gamma_\alpha$ can be replaced with the infinitesimal part $i\eta$, the retarded Floquet Green’s function becomes

$$\text{Im} \left( G_{r,\alpha,\alpha}(\mathcal{E}) \right) = \sum_{m=-\infty}^{\infty} \sum_\alpha \left| \phi^{(m-n)}_\alpha \right\rangle \langle \phi^{(m)}_\alpha | \mathcal{E} - m\Omega - E_\alpha + i\eta.$$ (4.4.5)

If we then consider the definition in Eq. (4.4.3) we get:

$$-\frac{\text{Im} \left( G_{r,\alpha,\alpha}(0) \right)}{\pi} = \sum_{m=-\infty}^{\infty} \sum_\alpha \left| \phi^{(m)}_\alpha \right\rangle \langle \phi^{(m)}_\alpha | \delta(\mathcal{E} - m\Omega - E_\alpha + i\eta).$$ (4.4.6)

We see that this quantity contains delta functions with peaks at the eigenenergies of each sidebands. Therefore it contains information on how the different sidebands are weighted. Here we considered the non-dissipative case but the definition holds equally well in that case. This Green’s function component generalize the notion of density of states and spectral function to periodically driven systems. To get the total density of states of the system the trace is taken over the imaginary part of the 0’th component of the retarded Floquet Green’s function. If only a subsystem is considered then the individual diagonal components corresponding to the sites in this subsystems are summed up. The quantities defined here allow us analyze the density of both finite systems and even semi-infinite systems such as the ribbons introduced in Chapter 3. With these quantities we may for instance check how the sidebands of edge states carry different weight. We will discuss this further later.

### 4.4.2 Time-averaged particle- and current density

The quantization of conductance through Chern insulators in two terminal configurations is one of the key signatures of these systems. However there are other local quantities that can also be obtained to check that transport really is mediated by edge states alone. In turns out that Green’s functions also provides a route to obtain such quantities. Therefore we now set out to find the particle density of the steady state system. We will be interested in time averaged particle density, since we are not dealing with stationary states. We define the time-averaged particle density in the site basis as [42]

$$\langle \langle n_i(t) \rangle \rangle = \frac{1}{T} \int_0^T dt \langle n_i(t) \rangle = \frac{1}{T} \int_0^T dt \langle c_i^\dagger(t) c_i(t) \rangle = -\frac{i}{T} \int_0^T dt \langle G^< (t,t) \rangle_{i,i}.$$ (4.4.7)
A detailed calculation of how to find the lesser Green’s function in the steady state and derive an expression for the density is found in Appendix B.8 where we obtain

$$
\langle \langle n_i(t) \rangle \rangle = \frac{1}{2\pi} \sum_{\nu=-\infty}^{\infty} \int_{-\infty}^{\infty} dE \left[ f_L(E) \left( G^{r(n)}(\epsilon) \Gamma_L \left( G^{r(n)}(\epsilon) \right)^\dagger \right)_{i,i} + f_R(E) \left( G^{r(n)}(\epsilon) \Gamma_R \left( G^{r(n)}(\epsilon) \right)^\dagger \right)_{i,i} \right].
$$

(4.4.8)

where we imposed the wide-band limit. Besides the net current in the system it would be nice to know how the current runs locally inside the system. Such a current density can conveniently be obtained via the current operator, which is given by [37, 42]:

$$
J_{ij}(t) = \frac{\delta H}{\delta (A(t))_{ij}},
$$

(4.4.9)

where $J_{ij}(t)$ is the current running from site $i$ to $j$ and $\frac{\delta}{\delta (A(t))_{ij}}$ denotes the functional derivative with respect to the local magnetic vector potential $(A(t))_{ij}$. For the graphene system in Eq. (3.3.1) the magnetic vector potential is given by $(A(t))_{ij} = A(t) \cdot (r_j - r_i)$. Just like for the net current, we will consider the current density over one time period. By taking the time average and the expectation value, one obtains the following expression for the current density of the graphene system

$$
\langle \langle J_{ij}(t) \rangle \rangle = -\frac{e}{\hbar T} \int_0^T dt \left( J_{ij}(t)G_{ij}^\ast(t, t) + (J_{ij}(t))^\ast \left( G_{ij}^\ast(t, t) \right)^\ast \right) = -\frac{e^2}{\hbar T} \int_0^T dt 2 \text{Re} \left( J_{ij}(t)G_{ij}^\ast(t, t) \right).
$$

(4.4.10)

The details can be found in Appendix B.9 where an expression for the current density above is found. In the steady state the time-averaged current density becomes

$$
\langle \langle J_{ij}(t) \rangle \rangle = \frac{2e}{\hbar} \sum_{m,n=-\infty}^{\infty} \int_{-\infty}^{\infty} dE \text{Im} \left[ \left( G^{r(m)}(\epsilon) \Gamma_L \left( G^{r(m)}(\epsilon) \right)^\dagger \right)_{i,j} J_{\rho(m-n)}(\lambda) e^{i\rho(m-n)(\frac{\pi}{2} - \phi_{ij})} + \left( G^{r(m)}(\epsilon) \Gamma_R \left( G^{r(m)}(\epsilon) \right)^\dagger \right)_{i,j} f_R(E) J_{\rho(m-n)}(\lambda) e^{i\rho(m-n)(\frac{\pi}{2} - \phi_{ij})} \right]
$$

(4.4.11)

where the effective hopping parameter $J_{\rho(m-n)}(\lambda)$ is given by $J_{\rho(m-n)}(\lambda) = J_{\lambda} J_{\rho(m-n)}(\lambda)$. Here $J_{\rho(m-n)}(\lambda)$ denotes the Bessel function of the first kind of order $\rho(m-n)$ with $\rho = \pm 1$ being the chirality of the drive and $\lambda = \frac{\alpha A_n}{\hbar}$.

### 4.4.3 non-equilibrium distribution function

For equilibrium topological insulators their distribution function is a priori known. When contacts are applied one has to deal with a non-equilibrium problem. Following the argument by Buttiker, it was argued in section 3.2.1 that if one only consider a bias window that matches the gap in a Chern insulator, the conductance will be quantized in units of

$$
2\pi f(\epsilon) \rho_i(\epsilon),
$$

(4.4.12)

where $\rho_i(\epsilon) = \delta(\epsilon - \epsilon_i)$ is the local density of states and $f(\epsilon)$ is the equilibrium distribution function which for fermions is just the Fermi-Dirac distribution. The total density of states can be obtained by
we use a similar candidate namely the 0'th component of the retarded Floquet Green’s function that was the relevant quantity. Here of Eq. (4.4.12) for periodically driven systems. For the time averaged density of states we saw that it is not straightforward to see that this gives us the non-equilibrium distribution function. However this guess is a good starting point, as we will see shortly. First however we need to find the correct analogue of Eq. (4.4.12) for periodically driven systems? A naive guess would be to repeat the procedure above using Floquet Green’s functions, but it is not straightforward to see that this gives us the non-equilibrium distribution function. However this guess is a good starting point, as we will see shortly. First however we need to find the correct analogue of Eq. (4.4.12) for periodically driven systems. For the time averaged density of states we saw that it was the 0'th component of the retarded Floquet Green’s function that was the relevant quantity. Here we use a similar candidate namely

\[ G^{(0)}(\mathcal{E}) = \frac{1}{T} \int_0^T dt G^<(t, \mathcal{E}) = \frac{1}{T} \int_0^T dt \int_{-\infty}^{\infty} dt' e^{\mathcal{E}(t-t')} G^<(t, t'). \]  

(4.4.16)

In Appendix B.10 the integrals are carried out in detail. Here we state the result

\[ G^<(0)(\mathcal{E}) = i \sum_{n=-\infty}^{\infty} \left( G^{(n)}(\mathcal{E} - n\Omega) f_L(\mathcal{E} - n\Omega) \Gamma_L(\mathcal{E} - n\Omega) \left( G^{(n)}(\mathcal{E} - n\Omega) \right)^\dagger + G^{(n)}(\mathcal{E} - n\Omega) f_R(\mathcal{E} - n\Omega) \Gamma_R(\mathcal{E} - n\Omega) \left( G^{(n)}(\mathcal{E} - n\Omega) \right)^\dagger \right). \]  

(4.4.17)

This result actually has a natural physical interpretation that hints that it might tell us about the system occupation. Each term describes an electron that goes into the system at left/right lead via \( \Gamma_{L,R}(\mathcal{E} - n\Omega) \) at energy \( \mathcal{E} - n\Omega \). The electrons then propagate around at this energy while they absorb/emit \( n \) photons such that they end up at energy \( \mathcal{E} \). This is described by the Green’s functions \( G^{(n)}(\mathcal{E} - n\Omega) \) and \( (G^{(n)}(\mathcal{E} - n\Omega))^\dagger \). Like for the conductance both the retarded Floquet Green’s function and its hermitian conjugate are needed since propagation for each photon index \( n \) is a probabilistic event and therefore involves some probability which is related to the modulus squared of the Floquet Green’s function. The sum over different photon absorption and emission events then adds up the probability of all these events. Since the electrons all end up at energy \( \mathcal{E} \) this hints that the lesser Green’s function at energy \( \mathcal{E} \) contains information on the occupation of the driven system at this energy. To get additional evidence that this quantity relates to the occupation of the system we will now relate it to the time averaged particle density. We start by going to the wide-band limit and then take the imaginary part on both sides of Eq. (4.4.17) to get

\[ \text{Im} \left( G^{(0)}(\mathcal{E}) \right) = \sum_{n=-\infty}^{\infty} \left( G^{(n)}(\mathcal{E} - n\Omega) \Gamma_L \left( G^{(n)}(\mathcal{E} - n\Omega) \right)^\dagger f_L(\mathcal{E} - n\Omega) + G^{(n)}(\mathcal{E} - n\Omega) \Gamma_R \left( G^{(n)}(\mathcal{E} - n\Omega) \right)^\dagger f_R(\mathcal{E} - n\Omega) \right). \]  

(4.4.18)
we now integrate this term over energy to get

\[
\int_{-\infty}^{\infty} d\mathcal{E} \text{Im} \left( G^{<}(0)(\mathcal{E}) \right) = \int_{-\infty}^{\infty} d\mathcal{E} \sum_{n=-\infty}^{\infty} \left( G^{r}(n)(\mathcal{E} - n\Omega)\Gamma_{L} \left( G^{r}(n)(\mathcal{E} - n\Omega) \right)^{\dagger} f_{L}(\mathcal{E} - n\Omega) \\
+ G^{r}(n)(\mathcal{E} - n\Omega)\Gamma_{R} \left( G^{r}(n)(\mathcal{E} - n\Omega) \right)^{\dagger} f_{R}(\mathcal{E} - n\Omega) \right)
\]

\[
= \int_{-\infty}^{\infty} d\mathcal{E} \sum_{n=-\infty}^{\infty} \left( G^{r}(n)(\mathcal{E}')\Gamma_{L} \left( G^{r}(n)(\mathcal{E}') \right)^{\dagger} f_{L}(\mathcal{E}') + G^{r}(n)(\mathcal{E}')\Gamma_{R} \left( G^{r}(n)(\mathcal{E}') \right)^{\dagger} f_{R}(\mathcal{E}') \right),
\]

(4.4.19)

where the change of variable \( \mathcal{E}' = \mathcal{E} - n\Omega \) was performed in the last line. By comparing with the result for the particle density in Eq. (4.4.8) we see that:

\[
\langle n_{i}(t) \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\mathcal{E} \text{Im} \left( G^{<}(0)(\mathcal{E}) \right).
\]

(4.4.20)

As it turns out our the guess actually has a physical meaning. By integrating up the 0’tth harmonic of the lesser Green’s function we get the particle density. Now if take the trace of both sides in the equation above we get

\[
\langle n(t) \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\mathcal{E} \text{Tr} \left[ \text{Im} \left( G^{<}(0)(\mathcal{E}) \right) \right].
\]

(4.4.21)

By comparing this with Eq. (4.4.15) we see that the lesser Floquet Green’s function \( G^{<}(0)(\mathcal{E}) \) seem to have the same property as the equilibrium lesser Green’s function. For this reason we define the non-equilibrium distribution \( \tilde{f}(\mathcal{E}) \) function as:

\[
\tilde{f}(\mathcal{E}) = \frac{1}{2\pi} \text{Tr} \left[ \text{Im} \left( G^{<}(0)(\mathcal{E}) \right) \right] = \frac{1}{2\pi} \text{Tr} \left[ \text{Im} \left( G^{<}(0)(\mathcal{E}) \right) \right] - \frac{1}{2\pi} \text{Tr} \left[ \text{Im} \left( G^{r}(0)(\mathcal{E}) \right) \right].
\]

(4.4.22)

Here the trace can be over any subset of the system, but of course the same trace has to be carried out in both denominator and numerator. For instance one might want to check the non-equilibrium distribution function at the edge or bulk only.

Now that the formalism of Green’s functions have been developed all that remains is to implement the formalism numerically. It turns out that additional methods are necessary since the computation time quickly becomes to large if one applies the formalism developed in this chapter directly. Therefore the next chapter in this thesis is devoted to the description of an efficient numerical algorithm for Floquet Green’s functions.
Chapter 5

Numerical technique for non-equilibrium Green’s functions

In the previous chapter the necessary machinery to numerically analyze transport through periodically driven systems was introduced. Although numerically solving these equations is in principle straightforward it is not very efficient. The problem is the time it takes to perform numerical computations. The step that takes up time is matrix inversion\(^1\). Numerically inverting large matrices by brute force is generally impractical since the time it takes to perform an inversion grows rapidly with the size of the matrix in question. This problem manifests itself when we are trying to compute Green’s functions using the method described in previous chapter. Here the size of the matrices are determined from the size of the mesoscopic system we are dealing with. The time it takes to compute Green’s functions using a brute force approach scales cubically with the size of the tight-binding Hamiltonian. In one dimension this means that the computation time is of order \(O(L^3)\) where \(L\) is the length of the system. Similarly in two dimensions the computation time is of the order \(O((W \times L)^3)\), where \(L\) is again the length of the system and \(W\) is the width of the system. The problem is even bigger when we are dealing with periodically driven systems. When we are computing Floquet Green’s functions we are applying the extended space formalism introduced in 4.2.1. Besides the physical dimensions of the system there are additional \(2M+1\) copies such that the computation time is of order \(O(((2M+1) \times L)^3)\) and \(O(((2M+1) \times W \times L)^3)\) in one and two dimensions respectively. Therefore we wish to find a more numerically feasible method while still maintaining a high numerical accuracy. There exist several computational methods that are designed specifically to obtain Green’s function in mesoscopic systems. For the results produced in this thesis we have chosen the Recursive Green’s function (RGF) technique which is introduced in this chapter.

5.1 The recursive Green’s function technique

The idea behind the Recursive Green’s function technique is the following [43]. Suppose we have a finite two dimensional system connected to two external leads. We already know how to compute Green’s functions for this system using the brute force approach. The idea behind the RGF algorithm is to divide the system into smaller parts so called slices, see Fig. 5.1. Instead of writing down the Hamiltonian for the entire system we instead define Hamiltonians for each slice in the system as well as matrices that describe hopping between slices. The idea is then to find different matrix elements of the full Green’s function by first performing inversion on smaller subsystems separately. Since the size of a slice is much smaller than the size of the system this algorithm is faster than brute force inversion. The reasoning behind this strategy is that for a non-interacting system the only thing that can influence some small part of a large system is how particles can diffuse between the subsystem and the surrounding system. In chapter 4 we saw that the only thing that separates the bare Green’s function of a non-interacting isolated system coupled to external baths from the Green’s function of a non-interacting isolated system is the coupling between the external baths. In the language of Green’s functions this is described by the Dyson equation:

\[
G^r = G^r_0 + G^r_0 \Sigma^r G^r
\]  

(5.1.1)

In the same way that an external lead acts as a bath for the full system, each slice can be regarded as a subsystem with its adjacent slices acting as external baths. The idea is then that the full Green’s

\(^1\)What most people do is actually numerical Gaussian elimination since this is faster and numerically stable.
function for a given slice in the system can be determined using a Dyson equation like the one in Eq. (5.1.1) but for Green’s functions describing just one slice. The bare Green’s function is then simply the Green’s function for the slice alone as if it was disconnected from the rest of the system. The self energy will describe how different slices are connected to neighboring slices as well as the external leads. For a tight-binding model this is simply determined by the hopping parameters between sites on different slices as well as on site potentials and hopping parameters between sites on the same slice. In order to obtain these Green’s functions however it turns out that it is useful to first define a different type of Green’s function. We now consider a physical picture similar to the one in Fig. 5.1. However this time we are working with an artificial system similar to the actual system. We assume that the artificial system is not fully constructed yet. Instead we consider a setup with only two baths, the left lead and the first slice of the system, see Fig. 5.2a. The first step is then to compute Green’s functions for this two piece system. We will subsequently add an extra slice and compute Green’s functions again. We continue to do so until the artificial system has \( N - 1 \) slices, where \( N \) is the number of slices in the actual physical system we are interested in. It will become clear later that only \( N - 1 \) slices are needed although it seems strange at first sight. We refer to the Green’s functions we compute from this artificial system as left Green’s functions \( G^L \). There is no a priori reason why this is a good idea in the first place. However as we shall see the left Green’s functions are building blocks that can be used to obtain the actual Green’s functions of the system. We will now see how this works in detail. We start with a configuration with only the left lead and the first slice, like depicted in Fig. 5.2a. The full left Green’s function for this two slice system satisfies the Dyson equation:

\[
G^L = G^{L,0} + G^{L,0} \Sigma G^L.
\]  

Here the bare Green’s function of the two slice system is simply the sum of the Green’s function of each individual slice without any coupling to an external slice:

\[
(G^{L,0})_{ij} = |L\rangle \langle L| (g_L)_{ij} + |1\rangle \langle 1| (g_1)_{ij},
\]  

Here \( g_L \) denotes the Green’s function for the left lead alone and \( g_1 \) denotes the Green’s function for the first slice alone. The projectors are onto the left lead and the first slice respectively. The superscripts on the Green’s functions denote the type of Green’s function and the subscripts denote the slice index. The indices \( i \) and \( j \) are site indices. The Green’s function \( g_\alpha \) for the \( \alpha \)’th slice in the system is given by:

\[
g_\alpha = \frac{1}{\mathcal{E} - h_\alpha + i\epsilon},
\]
where $\mathcal{E}$ denotes the energy and $h_\alpha$ is the Hamiltonian for the $\alpha$th slice. The parameter $\epsilon$ is an infinitesimally small parameter which is present to ensure that $g_\alpha$ has the correct analytic structure [37]. The self energy determines how the slice and the lead are coupled together. For a two slice system the self energy only has two terms
\[
(\Sigma)_{ij} = |L\rangle \langle 1| (V_{L,1})_{ij} + |1\rangle \langle L| (V_{1,L})_{ij}.
\] (5.1.5)
Here the matrices $V_{L,1}$ and $V_{1,L}$ describe how each site in the first slice is coupled the lead $L$. We recognize it as the matrix we used in section 4.3.1 when we derived the Jauho Wingreen Meir formula for the current. From the hermicity of the Hamiltonian it follows that $V_{L,1} = V_{1,L}^\dagger$. The full left Green’s function for the first slice is then given by:

\[
(G^L_{1,1})_{ij} = (g_{1,1})_{ij} + \sum_{k,l} \sum_{m,m'} (1) (G^0)_{ik} |m\rangle \langle m| (\Sigma)_{kl} |m'| \langle m'| (G^L)_{lj} |1\rangle
\] (5.1.6)

In matrix form the equation reads

\[
G^L_{1,1} = g_{1,1} + g_{1,1} V_{1,L} G^L_{L,1}.
\] (5.1.7)

To get a closed expression for $G^L_{1,1}$ we compute $G^L_{L,1}$

\[
(G^L_{L,1})_{ij} = (g_{1,1})_{ij} + \sum_{m,m'} \langle L| (G^{L,0})_{ik} |m\rangle \langle m| (\Sigma)_{kl} |m'| \langle m'| (G^L)_{lj} |1\rangle
\]

\[
= \sum_{k,l} (g_{l})_{ik} (V_{1,L})_{kl} (G^L_{1,1})_{lj} \iff G^L_{L,1} = g_{l} V_{1,L} G^L_{1,1}.
\] (5.1.8)

Inserting Eq. (5.1.8) into Eq. (5.1.7) we then get:

\[
G^L_{1,1} = g_{1,1} + g_{1,1} V_{1,L} g_{L} V_{L,1} G^L_{1,1}
\]

\[
\iff (1 - g_{1,1} V_{1,L} g_{L} V_{L,1}) G^L_{1,1} = g_{1,1}
\]

\[
\iff g_{1,1} (g^{-1}_{1,1} - V_{1,L} g_{L} V_{L,1}) G^L_{1,1} = g_{1,1}
\]

\[
\iff G^L_{1,1} = (g^{-1}_{1,1} - V_{1,L} g_{L} V_{L,1})^{-1}.
\] (5.1.9)

The term $V_{1,L} g_{L} V_{L,1}$ is the first entries in the retarded self energy $\Sigma^r$ we encountered in section 4.3.1. We argued that in the wide band limit this is simply given by the matrix $-i\Gamma^r_L$. Using the wideband limit and the expression for the bare Green’s function of the first slice in Eq. (5.1.4) we can write the left Green’s function in Eq. (5.1.9) as

\[
G^L_{1,1} = \left(\mathcal{E} - h_{1,1} + \frac{i\Gamma^r_L}{2}\right)^{-1}.
\] (5.1.10)

Here we neglected the infinitesimal part from Eq. (5.1.4) since the self energy carries a finite imaginary part by itself. If the algorithm is to be used without external contacts however an infinitesimal part must always be included. The left Green’s function $G^L_{1,1}$ fully describes the combined lead-slice system. In order for the algorithm to work we have assumed that the left (right) contact only couples to the first (last) site in the system. This is not very restrictive however since contacts are typically only connected to first few slices of a system in experiments. We now add an additional slice to the existing system from the right. The bare Green’s function for this new two slice system is then the sum of the left Green’s function $G^L_{1,1}$, which describes combined two slice system containing the left lead and the first slice, and the Green’s function of the isolated second slice $g_2$:

\[
G^{L,0} = |1\rangle \langle 1| G^L_{1,1} + |2\rangle \langle 2| g_2.
\] (5.1.11)

This situation is depicted in Fig. 5.2b. Once again the self energy describes how the two slices are coupled together

\[
\Sigma = |2\rangle \langle 1| V_{2,1} + |1\rangle \langle 2| V_{1,2}.
\] (5.1.12)
Here the matrices $V_{1,2}$ and $V_{2,1}$ are simply matrices that contain the nearest neighbor hopping parameters between each site in the first slice and its neighbor in the second slice. In order to obtain the full Green’s function of the second slice given that it is coupled to the first slice, we use Eqs. (5.1.11), (5.1.12) and (5.1.2). We then obtain:

$$
(G_{2,2}^L)_{ij} \equiv \langle (2|G_{1}^L|2) \rangle_{ij}
$$

$$
= \langle (2|G_{L,0}^L|2) \rangle_{ij} + \sum_{k,l} \sum_{m,m'} \langle (2|G_{L,0}^L|m) \rangle_{ik}(\langle m|\Sigma|m'\rangle)_{kl}(\langle m'|G_{L}^L|2 \rangle)_{lj}
$$

$$
= (g_2)_{ij} + \sum_{k,l} (g_2)_{ik}(V_{2,1})_{kl}(G_{1,2}^L)_{lj} \iff G_{2,2}^L = g_2 + g_2V_{2,1}G_{1,2}^L.
$$

To obtain a closed expression for $G_{2,2}^L$ we first find a similar equation for $G_{1,2}^L$:

$$
(G_{1,2}^L)_{ij} \equiv \langle (1|G_{1}^L|2) \rangle_{ij}
$$

$$
= \sum_{k,l} \sum_{m,m'} \langle (1|G_{L,0}^L|m) \rangle_{ik}(\langle m|\Sigma|m'\rangle)_{kl}(\langle m'|G_{L}^L|2 \rangle)_{lj}
$$

$$
= \sum_{k,l} (G_{1,1}^L)_{ik}(V_{1,2})_{kl}(G_{1,2}^L)_{lj} \iff G_{1,2}^L = G_{1,1}^LV_{1,2}G_{1,2}^L.
$$

The expression for $G_{2,2}^L$ then reads:

$$
G_{2,2}^L = g_2 + g_2V_{2,1}g_1V_{1,2}G_{1,2}^L.
$$

We then obtain a closed expression for $G_{2,2}^L$:

$$
G_{2,2}^L = (g_2(g_2^{-1} - V_{2,1}G_{1,1}^LV_{1,2}))^{-1} g_2 = (g_2^{-1} - V_{2,1}G_{1,1}^LV_{1,2})^{-1} = (\mathcal{E} - h_2 - V_{2,1}G_{1,1}^LV_{1,2})^{-1},
$$

where it was used that $(AB)^{-1} = (B)^{-1}(A)^{-1}$. The Green’s function above still has a finite imaginary part since this carries over from $G_{1,1}^L$. The Green’s function $G_{2,2}^L$ now governs the external lead and the two slices. Next step would be to add a third slice and repeat the computational procedure see Fig. 5.2c. This iterative process can be repeated by adding new slices and computing new left Green’s functions until the artificial system has $N-1$ slices. Where $N$ is the number of slices contained in the actual physical system we wish to describe. The left Greens function for the $N-1$’th slice is given by:

$$
G_{N-1,N-1}^L = (\mathcal{E} - hN_1 - V_{N-1,N-2}G_{N-2,N-2}^GV_{N-2,N-1})^{-1}.
$$

Our motivation for obtaining the left Green’s function was that it is a building block for the Green’s
function of the actual system $G$. It turns out there is an additional ingredient required to obtain the full Green’s function. Above we only considered a system being build up from the left. We now build a new artificial system this time starting from the right lead. We start by considering a system with a right lead. We now add one slice which we will denote as the $N$’th slice. We can then define right Green’s functions $G^R$ for this new artificial system. Computing the right Green’s function for the $N$’th slice is straightforward. We simply need to iterate the procedure for the left Green’s function only starting from the right. The Dyson equation for the right lead and $N$’th slice is

$$G^R = G^{R,0} + G^{R,0} \Sigma G^R.$$  

(5.1.18)

The bare Green’s function is given by

$$(G^{R,0})_{ij} = |R\rangle \langle R| (g_R)_{ij} + |N\rangle \langle N| (g_N)_{ij},$$  

(5.1.19)

and self energy is

$$(\Sigma)_{ij} = |N\rangle \langle R| (V_{N,R})_{ij} + |R\rangle \langle N| (V_{R,N})_{ij}.$$  

(5.1.20)

By a computation completely similar to the one for the left Green’s function we obtain the right Green’s function for the $N$’th slice

$$G^R_{N,N} = (\mathcal{E} - h_{N,N} + \frac{i\Gamma_R}{2})^{-1}.$$  

(5.1.21)

We can now add the $N-1$’th slice and compute the right Green’s function $G^R_{N-1,N-1}$ in analogy with what was done for the artificial system starting from the left. For the new two slice system we define the bare Green’s function

$$(G^{R,0})_{ij} = |N\rangle \langle N| (G^{R,N,N})_{ij} + |N-1\rangle \langle N-1| (g_{N-1,N-1})_{ij},$$  

(5.1.22)

and the self energy

$$(\Sigma)_{ij} = |N\rangle \langle N-1| (V_{N,N-1})_{ij} + |N-1\rangle \langle N-1| (V_{N-1,N-1})_{ij}.$$  

(5.1.23)

We can then compute

$$G^R_{N,N-1} = G^R_{N,N} V_{N,N-1} G^R_{N-1,N-1},$$  

(5.1.24)

and

$$G^R_{N-1,N-1} = g_{N-1} + g_{N-1} V_{N-1,N} G^R_{N,N-1}.$$  

(5.1.25)

We can then obtain a closed expression for $G^R_{N-1,N-1}$:

$$G^R_{N-1,N-1} = (\mathcal{E} - h_{N-1} - V_{N-1,N} G^R_{N,N} V_{N,N-1})^{-1}.$$  

(5.1.26)

We can now iterate this procedure until we have the right Green’s function $G^R_{2,2}$:

$$G^R_{2,2} = (\mathcal{E} - h_{2,2} - V_{2,3} G^R_{3,3} V_{3,2})^{-1}.$$  

(5.1.27)

We won’t need the right Green’s function $G^R_{1,1}$ for the same reason we didn’t need $G^L_{N,N}$. These Green’s functions are simply not necessary to compute the actual Green’s functions for the system as we will see shortly.

We now consider the actual physical system like the one in depicted in Fig. 5.1. As a first step we wish to compute the full Green’s functions for each slice $G_{n,n}$. We have to keep in mind that now the $n$’th slice has an adjacent slice to the right as well as to the left. if we assume all slices to the left including the left lead is just one big slice and similarly that all slices to the right including the right lead is one big slice we have boiled the problem down to one slice with two baths. We can still write up a Dyson equation like the one presented in Eq. (5.1.2):

$$G = G^0 + G^0 \Sigma G.$$  

(5.1.28)

This time there are three pieces to the bare Green’s function. There is the Green’s function for the $n$’th slice itself $g_n$ as usual. Furthermore there is the Green’s function for all the slices to the left of the $n$’th slice. But this Green’s function is simply $G^L_{n-1,n-1}$ which we already know. Similarly the Green’s
function for all the slices to the right of the \( n \)'th slice is \( G_{n+1,n+1}^R \). Taking this into account the bare Green’s function is given by:

\[
(G^0)_{ij} = |n\rangle \langle n| (g_{n})_{ij} + |n-1\rangle \langle n-1| (G_{n-1,n-1}^L)_{ij} + |n+1\rangle \langle n+1| (G_{n+1,n+1}^R)_{ij},
\]

and the potential is given by

\[
(S)_{ij} = |n\rangle \langle n-1| (V_{n,n-1})_{ij} + |n\rangle \langle n+1| (V_{n,n+1})_{ij} + |n-1\rangle \langle n-1| (V_{n-1,n})_{ij} + |n+1\rangle \langle n+1| (V_{n+1,n})_{ij},
\]

We now compute \( G_{n,n} \):

\[
(G_{n,n})_{ij} = (g_{n})_{ij} + \sum\sum (|n\rangle \langle m| G^0_{ij} |m\rangle \langle m'| |m'| \Sigma |m\rangle |G|)_{ij} = (g_{n})_{ij} + \sum\sum (|n\rangle \langle m| V_{n,n-1} |m\rangle \langle m'| |G_{n,n}|)_{ij}
\]

\( \iff \)

\( G_{n,n} = g_{n} + g_{n} (V_{n,n-1}G_{n,n} + V_{n,n+1}G_{n,n+1}) \)

To get a closed expression for \( G_{n,n} we first find \( G_{n-1,n} \) and \( G_{n+1,n} \):

\[
(G_{n-1,n})_{ij} \equiv (|n-1\rangle \langle n| G^0)_{ij} = \sum\sum (|n-1\rangle \langle m| G^0_{ij} |m\rangle \langle m'| |m'| \Sigma |m\rangle |G|)_{ij} \]

\( \sum\sum (G_{n-1,n}^L)_{ij} (V_{n,n-1})_{ij} \iff \)

\( G_{n-1,n} = G_{n-1,n}^L V_{n-1,n} G_{n,n} \)

\[
(G_{n+1,n})_{ij} \equiv (|n+1\rangle \langle n| G^0)_{ij} = \sum\sum (|n+1\rangle \langle m| G^0_{ij} |m\rangle \langle m'| |m'| \Sigma |m\rangle |G|)_{ij} \]

\( \sum\sum (G_{n+1,n}^R)_{ij} (V_{n,n+1})_{ij} \iff \)

\( G_{n+1,n} = G_{n+1,n}^R V_{n+1,n} G_{n,n} \)

With this set of equations we can now find a closed expression for \( G_{n,n} \):

\[
G_{n,n} = g_{n} + g_{n} (V_{n,n-1}G_{n-1,n}^L V_{n-1,n} G_{n,n} + V_{n,n+1}G_{n+1,n}^R V_{n+1,n} G_{n,n})
\]

\( \iff \)

\[
(1 - g_{n} V_{n,n-1} G_{n-1,n}^L V_{n-1,n} - g_{n} V_{n,n+1} G_{n+1,n}^R V_{n+1,n} ) G_{n,n} = g_{n}
\]

\( \iff \)

\[
G_{n,n} = (E - h_{n,n} - V_{n,n-1} G_{n-1,n}^L V_{n-1,n} - V_{n,n+1} G_{n+1,n}^R V_{n+1,n})^{-1}. \)

It is now clear that the procedure of finding diagonal matrix elements of \( G^L \) and \( G^R \) is very convenient since these are building blocks of the matrix elements \( G_{n,n} \) of the actual system Green’s function. By inspecting Eq. (5.1.34) we see that for \( n = 1 \) and \( n = N \) respectively it looks like the Green’s functions \( G_{n-1,n-1}^L \) and \( G_{n+1,n+1}^R \) become ill-defined since the there are no \( n = 0 \) slice nor a \( n = N+1 \) slice. However we can think of these slices as the external leads. In these cases the Green’s functions are given by

\[
G_{1,1} = \left( E - h_{1,1} + i\frac{\Gamma_L}{2} - V_{1,2} G_{2,2}^R V_{2,1} \right)^{-1},
\]

\[
G_{N,N} = \left( E - h_{N,N} + i\frac{\Gamma_R}{2} - V_{N,N-1} G_{N-1,N-1}^L V_{N-1,N} \right)^{-1}.
\]

To confirm this picture a different but equivalent way to think about this is to say that the leads have been traced out, but that they still affect the system through the matrices \( -i\Gamma_{L/R} \). Therefore an equivalent approach to the one above is to modify the first and last slice Green’s functions as

\[
\tilde{g}_{1/N} = \frac{1}{E - h_{1/N} - i\frac{\Gamma_{L/R}}{2}}.
\]
By comparing this with the expressions in Eq. (5.1.10) and Eq. (5.1.21) we see that \( \tilde{g}_1 = G^L_{1,1} \) and \( \tilde{g}_N = G^R_{N,N} \). The bare Green’s function in this case is:

\[
G^0 = |1]\langle 1|G^L_{1,1} + |2]\langle 2|G^R_{2,2}.
\]

(5.1.38)

The reason this is more convenient is that a transmission coefficient in principle should be from left lead to the right lead. But to make to formalism here resemble that of the previous chapter it is more natural to have transport be from the first slice to the last slice. This is equivalent to the formalism of transmission probabilities where particular components of the Floquet Green’s functions are picked out. In particular this will be the sites coupled to external leads, which in the RGF language is just the first and last slice.

The quantities \( G_{n,n} \) obtained via the RGF technique correspond to blocks on the diagonal of the full system Green’s function that one normally obtains via inversion. In order to compute quantities such as the local density of states the diagonal components \( G_{n,n} \) are enough. However if we are interested in transport properties the on slice Green’s functions are not enough. For instance if we wish to compute the transmission probability the relevant Green’s functions are \( G_{1,N} \). This is a matrix that describes propagation between the first slice and the last. The \( ij \)’th entry is propagation from the \( i \)’th site in the first slice to the \( j \)’th site in the \( N \)’th slice. We use the Dyson equation to get:

\[
G_{1,N} = \sum_{m,m'} (|1]\langle m|G^0|m'\rangle \sum\langle m'|G|N\rangle = G^L_{1,1}V_{1,2}G_{2,N}.
\]

(5.1.39)

We perform a similar calculation for \( G_{2,N} \):

\[
G_{2,N} = \sum_{m,m'} (|2]\langle m|G^0|m'\rangle \langle m'|G|N\rangle = g_2(V_{2,1}G_{1,N} + V_{2,3}G_{3,N}).
\]

(5.1.40)

Using Eq. (5.1.39) we rewrite Eq. (5.1.40) as:

\[
G_{2,N} = g_2(V_{2,1}G^L_{1,1}V_{1,2}G_{2,N} + V_{2,3}G_{3,N})
\]

\[
\iff (1 - g_2V_{2,1}G^L_{1,1}V_{1,2}G_{2,N})G_{2,N} = g_2V_{2,3}G_{3,N}
\]

\[
\iff G_{2,N} = (g_2^{-1} - V_{2,1}G^L_{1,1}V_{1,2}G_{2,N})^{-1}V_{2,3}G_{3,N} = G^L_{2,3}V_{2,3}G_{3,N}.
\]

(5.1.41)

We can iterate the procedure above obtaining an expression for \( G_{3,N} \) in terms of \( G_{4,N} \) and so on. The final equation will be

\[
G_{N-1,N} = G^L_{N-1,N-1}V_{N-1,N}G_{N,N}.
\]

(5.1.42)

We can then insert this expression into the previously obtained one to get

\[
G_{N-2,N-1} = G^L_{N-2,N-2}V_{N-2,N-1}G^L_{N-1,N-1}V_{N-1,N}G_{N,N}.
\]

(5.1.43)

By reinserting each equation into the former the expression for \( G_{1,N} \) becomes:

\[
G_{1,N} = G^L_{1,1}V_{1,2}G^L_{2,2}V_{2,3}G^L_{3,3}\cdots V_{N-1,N}G_{N,N}.
\]

(5.1.44)

If we consider transport were the symmetry between left and right transmission is broken an additional Green’s function is needed namely \( G_{N,1} \). This can be computed in complete analogy with \( G_{1,N} \) only now the right Green’s functions are needed:

\[
G_{N,1} = G^R_{N,N}V_{N,N-1}G_{N-1,1}.
\]

(5.1.45)

By iterating this procedure one obtains:

\[
G_{N,1} = G^R_{N,N}V_{N,N-1}G^R_{N-1,N-1}V_{N-1,N-2}G^R_{N-2,N-2}\cdots G^R_{2,2}V_{2,1}G_{1,1}.
\]

(5.1.46)

This approach might seem tedious but it actually involves no additional matrix inversion. In chapter 4 we introduced physical observables that are also computed from Green’s functions. We already computed the Green’s functions \( G_{1,N} \) and \( G_{N,1} \). However we need additional Green’s functions \( G_{j,N} \) and \( G_{1,j} \), where \( j \) is any slice in the system except for 1 and \( N \), if we wish to compute the particle- and the current
density as well as the non-equilibrium distribution function. But we actually already know these quantities since they are obtained at each iteration in used to obtain Eqs. (5.1.44) and (5.1.46). Once we know \( G_{N-1,N} \) we can obtain \( G_{N-2,N} \) and so forth. The same thing goes for the matrix elements \( G_{N,j} \) with \( N > j \). This method exhausts the necessary matrix elements required in order to compute transmission probabilities, particle- and current densities as well as non-equilibrium distribution functions.

In the derivation above we assumed that the wide band approximation is valid. The technique can also be applied to systems where this isn’t the case. However in that case one needs to obtain Green functions for the leads at a given energy. There are various ways to do this depending on the problem one wishes to solve [43]. At first sight the RGF algorithm might seem complicated. After all several steps are needed before the actual Green’s function can be obtained. Furthermore obtaining non-diagonal components requires additional computations. However due to the scaling with system size the algorithm is still favorable. After all \((N-1)\) matrix inversions are required to obtain left and right Green’s functions. Then an additional \( N \) inversions to obtain the diagonal components of the actual Green’s function. Finally these different components need to be multiplied together correctly to obtain the Green’s functions \( G_{1,N} \) and \( G_{N,1} \). However since each inversion involves only one slice the computation time scales only cubically with the width of the system. Adding more slices will require more inversions, but the size of the matrices being inverted are the same. Therefore the computation time scales linearly with the length of the system. The RGF technique is very useful since the time it takes to execute the algorithm scales as \( W^3 \times L \). The time it takes to perform a brute force inversion to obtain the full Green’s function scales as \((W \times L)^3\) which is \( L^2 \) times slower. Furthermore the RGF technique is numerically stable, does not require a large amount of computer memory and allows for parallel computations.

5.1.1 RGF and driven systems

The RGF techniques provides a natural route to study periodically driven systems. This is because periodically driven systems can be analyzed using the extended space formalism introduced in sections 2.2 and 4.2.1. As previously discussed the driven system is analyzed as a time-independent system containing many copies which are then coupled together by the external driving field. For instance 1D systems simulated using 5 copies would equivalent to describing a 2D system with the width 5. The same principle applies to 2D systems however here each copy is itself a 2D system so the width we need to simulate will be the actual physical width \( W \) times \((2M+1)\), see Fig. 5.3. Therefore 2D simulations will generally take longer but the RGF technique is still much faster than the brute force approach. However
there is a difference between the Floquet Greens functions obtained using the RGF and the one using the brute force approach. When we obtained the equation of motion in section 4.2.1 we had to perform inversion with respect to the identity:

\[
\begin{pmatrix}
\vdots \\
0 \\
I \\
0 \\
\vdots
\end{pmatrix}.
\] (5.1.47)

In the RGF algorithm the identity enters from the relation \( gg^{-1} = I \). The generalization of this identity to multiple copies of the same system is however given by:

\[
\begin{pmatrix}
\vdots \\
I \\
I \\
\vdots
\end{pmatrix}.
\] (5.1.48)

Therefore naively applying the RGF algorithm using the matrix structure obtained in section 4.2.1 with the identity \( I_{\delta_n,0} \) won’t yield the correct result. The extended space approach is however still valid if we instead use a modified version of the equation of motion \([9]\). In the modified version one instead defines a matrix of Floquet Green’s functions such that the set of equations that needs to be solved have the matrix structure:

\[
\begin{pmatrix}
\vdots \\
(\mathcal{E} + \Omega)I \\
\mathcal{E}I \\
(\mathcal{E} - \Omega)I \\
\vdots
\end{pmatrix}
- \begin{pmatrix}
\vdots \\
\cdots \tilde{H}(0) \cdots \\
\cdots \tilde{H}(1) \cdots \\
\cdots \tilde{H}(-1) \cdots \\
\vdots
\end{pmatrix}
\times
\begin{pmatrix}
\vdots \\
G_{r(0)}(\mathcal{E}) \\
G_{r(1)}(\mathcal{E}) \\
G_{r(-1)}(\mathcal{E}) \\
G_{r(0)}(\mathcal{E}) \\
\vdots \\
\vdots \\
\vdots \\
\vdots \\
\vdots
\end{pmatrix} = \begin{pmatrix}
\vdots \\
I \\
I \\
I \\
\vdots
\end{pmatrix}.
\] (5.1.49)

There is a degree of redundancy to this approach however since each column contains the same amount of information. In principle once the middle column of the Floquet Green’s function matrix in Eq. (5.1.49) is known we have extracted all the information that equations of motion contain. However it is not clear how the RGF algorithm should be modified such that it contains the identity operator in Eq. (5.1.47). This operator only contains an identity with physical dimension of the system in the zero photon subspace. Therefore when we apply the RGF technique in order to find Floquet Green’s functions we actually use the matrix structure in Eq. (5.1.49) for a single slice however. This approach is still good and much faster than the brute force approach and therefore it is not an issue we will pursue any further.

The extension of the RGF algorithm as described above is not restricted to periodically driven systems. The copies could also represent different orbitals of the same site or copies of the same site with particles of opposite spin.
Chapter 6

Transport with- and without energy filtered leads

The results presented in this chapter are obtained by the author in collaboration with Mark S. Rudner and Netanel H. Lindner, and are being prepared for submission to a journal.

In this section transport quantities are numerically computed for the two terminal configuration introduced in Chapter 4. The focus is on the graphene model introduced in Chapter 3. First computations are done using wide-band leads. A deviation from the quantized conductance present in non-driven systems is found and this result is explained in terms of sidebands. We discuss a result recently obtained regarding so called sum rules for periodically driven systems. It is then argued that in principle quantized transport can be restored if the system can be controlled such that a single edge state sideband mediates the transport. A toy model of an energy filtered lead is introduced and a modified two terminal setup is presented. The conductance for the modified system is found and compared to that of the non-filtered setup. Numerical results for the particle- and current densities are subsequently found and they are in good agreement with the results for the conductances. In addition non-equilibrium distribution functions are found for the graphene system with and without energy filtering leads. Finally we discuss the limitations of our results as well as possible implementations of energy filtered leads in transport experiments.

Throughout all numerical computations the following physical constants are set to 1: the electron charge $e$, Planck’s reduced constant $\hbar$, the lattice constant of graphene $a$. Throughout the chapter the of light polarization in any external drive used is chosen such that the parameter $\rho$ used to define the magnetic vector potential present in Eq. (3.3.1) is equal to one.

6.1 Transport without energy filtered leads

We start by analyzing transport through a Floquet topological insulator with wide-band leads. To do so we apply the formalism introduced in Chapter 4 and the numerical technique explained in Chapter 5 to the graphene model introduced in Eq. (3.3.1). The graphene model will act as the mesoscopic region in the two terminal configuration introduced in Eq. (4.1.1). We will then use this setup to numerically calculate time-averaged differential conductances and thereby highlight some of the issues associated with using wide-band leads for transport through periodically driven systems. The Hamiltonians considered are real space Hamiltonians for which the extended space formalism can be applied. As explained in section 2.2 the problem is mapped to a $(2M + 1) \times \text{dim}(\mathbb{R})$ dimensional problem, where $\mathbb{R}$ denotes the physical dimension of the system, and $M$ is a finite natural number that characterize how many copies are kept. We refer to it as the truncation parameter. The different extended space components of the graphene Hamiltonian in Eq. (3.3.1) can be found in Appendix C.1. The graphene geometry used is depicted in Fig. 6.1. Before any numerical results are presented we first discuss how the system and lead are coupled. As mentioned in Chapter 5 we consider a situation where the left (right) contact is only coupled to the first (last) slice in the system. All numerical computations in this chapter have been done using the same slicing scheme. It is depicted in Fig. 6.1. In the wideband limit these couplings are independent of energy. The couplings are chosen such that they couple to all sites on the same slice equally, that is each contact is characterized by a single coupling parameter $\Gamma_{L/R}$. We choose to work with symmetric couplings, that is both contacts have the same coupling parameter $\Gamma_L = \Gamma_R \equiv \Gamma$. This is typically what is done, since having asymmetric couplings generally leads to a lower conductance.
This can be seen by viewing the two terminal configuration as a transmission/reflection problem. In such a problem the interface between system and lead forms a barrier and the incoming electrons are waves that are either transmitted or reflected at the barrier. It can be shown that for symmetric barriers the conductance reaches its highest value [44]. Therefore the system-lead coupling is characterized by a single parameter. The value of this coupling parameter is chosen relative to the hopping parameter of the system $J_1$. We therefore write the coupling as $\Gamma = cJ_1$, where $c$ is some constant. We have found that there is a particular optimal coupling for which the differential conductance will assume its highest value. This can be understood from impedance matching \(^1\). Impedance matching plays a crucial role in many areas of physics. Here it can be understood in terms of waves. That is we think about the incoming electrons from the lead as a waves. The propagation of waves depends on the host medium. If a wave hits an interface between two different media, there is a certain probability that it is transmitted. Impedance matching means the interface barrier that results in the highest transmission probability. In the transport setup impedance matching boils down to choosing the correct system-lead coupling. By numerically varying the parameter $c$ it was found that $c = 1$ leads to the highest conductance and we therefore fix the parameter at this value for all computations.

\[\Gamma = cJ_1\]

Figure 6.1: Graphene geometry used in the two terminal setup. The slicing scheme used for numerical computations is indicated by the black box. The sites enclosed within the black rectangle forms a single slice.

The choice of system size for the numerical results presented here reflect the following considerations. As shown in section 3.2.2 the localization length of an edge state is inversely proportional to the topological mass gap of a given model. In our case the ratio between the driving amplitude and the driving frequency sets the size of the gap. For numerical simulations we will need a finite width. The width we will need to observe quantized transport therefore depends on the size of the gap. To small a gap will require a very large width which is not numerically realistic. Therefore the driving parameters also reflect this consideration. We have therefore chosen system widths large enough to see plateaus form in the conductance. In real experiments making a system wide enough is of course not a limitation. As for the system length it has to be large enough that quantum tunneling through the system is suppressed. Otherwise the signatures one might see won’t reflect transport associated edge states. Furthermore both system length and width has to be kept large enough that finite size effects do not occur.

The time-averaged differential conductance is calculated with the leads at zero temperature, by using the result found in Eq. (4.3.23). Before showing any results for periodically driven systems, we first obtain the differential conductance of a non-driven Chern insulator. As an example we choose the Haldane model introduced in section 3.3. The differential conductance for such a system can also be obtained by using Eq. (4.3.23), without the sum over different harmonics. This means only the transmission coefficients $T^0(E)$ are used. Results for this system allow us to compare the time-averaged differential conductance of Floquet topological insulators with those obtained for a non-driven Chern insulator. Furthermore it has served as a benchmark for the implementation of the RGF algorithm introduced in Chapter 5. In Fig. 6.2a a plot of the differential conductance through the two terminal

\(^1\)Impedance matching owes its name to the role it plays in the theory of electronic circuits.
setup using the Haldane model is shown. A system of length $L = 50$ and width $W = 81$ was used. The parameters chosen are: $J_1 = 1$, $J_2 = \frac{1}{4}$, $\phi = \frac{\pi}{2}$ and the inversion breaking mass $M$ is 0. This correspond to the topological regime of the Haldane model where it has one mode pr. edge. We obtain a plateau with perfectly quantized differential conductance as expected from the argument given in section 3.2.1.

![Figure 6.2](image.png)

Figure 6.2: a) Plot of the differential conductance for the Haldane model, in a finite geometry with $L = 50$ and $W = 81$. The model parameters used are $J_1 = 1$, $J_2 = \frac{1}{4}$, $\phi = \frac{\pi}{2}$ and the inversion breaking mass $M$ is 0. b) Plot of the time-averaged differential conductance of the graphene-model introduced in Eq. (3.3.1) in a finite geometry with $L = 50$ and $W = 81$. The model and drive parameters used are: $J_1 = 1$, $\Omega = 30$ and $\lambda = 1.4$.

We now compare the differential conductance obtained using the Haldane model with the time-averaged differential conductance of the driven graphene model in Eq. (3.3.1). We look at the model in the high frequency limit where a gap at $E = 0$ was predicted. Here direct photon assisted tunneling is not possible and therefore the conductance should still be quantized in units of $\frac{e^2}{h}$. A plot of the computed time-averaged differential conductance is depicted in Fig. 6.2b. Here the geometry used is identical to the one in the first figure with $L = 50$ and $W = 81$. The model and drive parameters used are $J_1 = 1$, $\Omega = 30$, $\lambda = 1.4$. The truncation parameter is $M = 2$. The parameters of the drive are far from what is realistic and were picked to make sure a sizable plateau would be visible. Therefore the results should merely serve to understand what happens to the conductance in the non-interacting model in the high-frequency limit. We see that the conductance is almost quantized but not quite. There can be several reasons for the deviation. One is that the effective Hamiltonian description is only good in the limit of very large frequency. Therefore one could always obtain a larger value of time-averaged differential conductance at $\mu = 0$ by choosing a larger frequency. This would also lead to a smaller gap and a larger system size would be needed. There is a limit to the width of systems for which numerical computation of the time-averaged differential conductance is possible. However the deviation could also be explained by results recently obtained [46]. We will postpone this discussion for a bit and turn our attention to the on-resonant driving regime.
Figure 6.3: a) Time-averaged differential conductance at the $E = 0$ for an on-resonant driving frequency. The parameters used are $L = 50$, $W = 81$, $J_1 = 1$, $\Omega = 3$ and $\lambda = 0.5$. b) Time-averaged conductance at the laser induced gap, which is centered around $E = 1.5$, for an on-resonant driving frequency. The system and drive parameters used are the same as in Fig. 6.3a.

We now study the on-resonant case. We focus on one photon resonances. To do so we use the driving frequency $\Omega = 3 J_1$. The full bandwidth of the graphene model is normally $6 J_1$. But the driven model is in fact described by the effective hopping parameter $J_{\text{eff}} = J_1 J(0)(\lambda)$ as explained in section 3.3.2. If we choose following parameters: $J_1 = 1$ and $\lambda = 0.5$, the effective system bandwidth is $D_{\text{system}} = 6 J(0)(\lambda) \approx 5.63$. Therefore only one photon absorption processes are possible at this driving frequency. In this parameter regime there are two gaps in the system bandwidth. One at $E = 0$ and one at $E = \frac{\Omega}{2}$. We checked the time-averaged differential conductance in both gaps. The systems sizes used are $L = 50$ and $W = 81$ for both gaps. The results are depicted in Figs. 6.3a and 6.3b. Unlike our previous results we don’t see quantization in integer units of $\frac{e^2}{h}$. In fact the sweep through the laser induced gap doesn’t even give a clear plateau but a line with a small slope is seen. The lack of quantization can in this case be understood in terms of photon assisted tunneling. Here the transmission probability at a given energy is determined from several processes. One is just that the electrons goes straight though without absorbing or emitting photons. Another is that an electron goes in absorbs one photon and the exits. Therefore several coefficients enter into the transmission probability in Eq. (B.7.36). These coefficients depend on the different retarded Floquet Green’s functions. These in turn is written in terms of different sidebands as seen in Eq. (4.2.33). The different sidebands are generally not on equal footing, in the sense that any Floquet state need not expanded in terms of equally weighted sidebands. Since different sidebands are shifted by integer values of $\Omega$, corresponding to absorption or emission of photons, the weight crucially depends on whether or not these processes are possible. In the off resonant case we saw almost perfect quantized conductance. Since photon absorption is not possible in that case, the transport of via the Floquet edge state $|\Phi_\alpha(t)\rangle$ is mediated by the sideband $|\phi_0^\alpha\rangle$ alone. To quantify the weight of sidebands we introduced the time-averaged density of states in Eq. (4.4.3). We will now find the time-averaged spectral function for the ribbon geometry introduced in section 3.3.2. In Fig. 6.4a the original bandstructure of the same ribbon geometry is depicted. This plot can also be found in Fig. 3.8a for a shorter quasienergy window. The ribbon used in Fig. 6.4a contained strips of consisting of 100 sites. The other parameters used are: $J_1 = 1$, $\Omega = 3$, $\lambda = 0.5$. In Fig. 6.4b the time averaged spectral function is depicted for the exact same system and drive parameters and the same resolution of momentum. The color intensity indicate the value of the spectral function $A^{(0)}(E)$ on a normalized scale. It is seen that sidebands of the edge states that are inside the energy window from $\{-\frac{\Omega}{2}, \frac{\Omega}{2}\}$ carry higher weight than those outside located at $\pm \Omega$. This indicates that in the on-resonant case the harmonics are not on equal footing like argued above. While the transport is through a finite sheet and not a ribbon, the same principle applies to the sidebands in the finite sheets. This is exactly what causes the differential conductance to deviate from the integer values of $\frac{e^2}{h}$ which is known for non-driven Chern insulators.
Figure 6.4: a) Floquet bandstructure for the graphene model in a ribbon geometry. For this plot the following parameters where used $J_1 = 1$, $\Omega = 3$ and $\lambda = 0.5$. Each strip contains 100 sites. b) The spectral function for a system with the same system and drive parameters as in Fig. 6.4a. The weight of the different sidebands fall of with increasing energy away from $E = 0$.

The lack of quantization seen here is quite general for transport through periodically driven topological systems. Recently it was shown that quantization in periodically driven systems can still be observed if one apply so called sum rules for the conductance [45, 46, 47, 42]. It was first shown by Kundu [45] for a one dimensional system that the sum of conductances on the form:

$$\tilde{G}(\mathcal{E}) = \sum_{n=-\infty}^{\infty} G(\mathcal{E} + n\Omega)$$  \hspace{1cm} \text{(6.1.1)}$$

is instead quantized. Here $G(\mathcal{E} + n\Omega)$ correspond to the conductance computed at some energy $\mathcal{E}$ like done above but shifted by an amount $n\Omega$, where $n$ is an integer. A similar rule was subsequently found for Chern insulators but for a toy model different than the one used here [46, 47]. There it was emphasized that in principle the sum rule also applies in the off resonant case. That is even at high frequency when photon-assisted tunneling shouldn’t be possible the sidebands $|\phi^{(n)}\rangle$ of some edge state, with $n$ an integer from zero, should still be included. In this case however the contribution from these sidebands is typically very small. We have numerically investigated this statement for the model used here in the off-resonant and the on-resonant case. The result is in good agreement with the statements in [46, 47]. These computations can be found in Appendix C.2. From a practical viewpoint the sum rule is not at all convenient. It implies that in order to measure quantized time-averaged differential conductance in an experiment one should not only measure the conductance at energy $\mathcal{E}$, but also at $\mathcal{E} + n\Omega$, where $n$ runs over all integers. Even if one considers a truncated sum it still means adding up many different measurements. This is difficult for periodically driven system since what is measured is already a time-averaged quantity meaning that for actual measurements a good time-resolved measurement technique is needed. Adding up several time-averaged measurements will therefore involve additional uncertainty. Therefore if it is possible to control the system in a way such that the only contribution to sum in Eq. (6.1.1) that of a single term, a quantized signature could in principle be obtained from a single time-averaged measurement. This is precisely what we hope an energy filtered lead might do, by blocking photon assisted tunneling such that $G(\mathcal{E} + n\Omega) \approx 0$ for $n \neq 0$.

### 6.2 Transport with energy filtered leads

We now add energy filtered leads into the two terminal setup. The filters are put between the periodically driven system and the wide band leads. This is modeled such that the filter is part of the system Hamiltonian. The time-dependent Hamiltonian now therefore has three parts

$$H(t) = H_{f1} + H_{\text{graphene}}(t) + H_{f2},$$  \hspace{1cm} \text{(6.2.1)}$$
where \( H_{f1} \) is the Hamiltonian for the first filter, \( H_{f2} \) is the Hamiltonian for the second filter and \( H_{\text{graphene}}(t) \) is the Hamiltonian in Eq. (3.3.1). The filters are identical, meaning that they are modeled from the same Hamiltonian and that they have the same size. The only difference being that one filter contains the first sites in the system and the second filter the last sites. To study the effect of using a filter for transport through periodically driven systems, we will be using a simple toy model. We have chosen the 2D square lattice with nearest neighbor hopping. This is a simple one band model which is exactly what an ideal energy filter has. The Hamiltonian for the filter is

\[
H_{\text{filter}} = J_f \sum_{\langle ij \rangle} \left( c_i^\dagger c_j + \text{h.c.} \right) \tag{6.2.2}
\]

where \( J_f \) is the nearest neighbor hopping parameter. The spectrum of this model is given by

\[
E(k_x, k_y) = 2J_f \left( \cos(k_x a) + \cos(k_y a) \right) \tag{6.2.3}
\]

where \( a \) is the lattice constant of the 2D square lattice. The bandwidth of this system is given by \( 8J_f \).

In order for the filter to work this bandwidth needs to be small compared to the driving frequency. The band of this model is centered around \( E = 0 \). This is good for checking the \( E = 0 \) gap but won’t allow us to check the \( E = \frac{\hbar \Omega}{2} \) gap. We wish to probe both gaps. Therefore we add an offset term to the system of the form \( -V_g I \). Here \( I \) denotes the identity matrix of the same dimension as the physical dimension of the driven system and \( V_g \) is a gate voltage. We choose this name for the parameter since a natural way to implement such a term is to put a gate underneath the driven system that can be used to control the position of the systems energy levels by tuning the gate voltage. In this way we can keep the 2 filters fixed and probe the time-averaged differential conductance in different gaps by sweeping over the gate voltage. The full system Hamiltonian then reads

\[
H(t) = J_f \sum_{\langle ij \rangle \in \text{filter}_1} \left( c_i^\dagger c_j + \text{h.c.} \right) + \sum_{\langle ij \rangle \in \text{system}} \left( J_{ij}(t) c_i^\dagger c_j + \text{h.c.} \right) - V_g \sum_{i \in \text{system}} c_i^\dagger c_i + J_f \sum_{\langle ij \rangle \in \text{filter}_2} \left( c_i^\dagger c_j + \text{h.c.} \right). \tag{6.2.4}
\]

The computation of retarded Floquet Green’s functions for this system are done with a slight modification. Now the retarded Floquet Green’s functions are computed at a fixed energy, but are functions of gate voltage \( G^{r(n)}(E, V_g) \). The energy has been fixed at \( E = 0 \) for all computations. When computing differential conductances this correspond to putting the external chemical potential \( \mu = 0 \).

Now that 3 subsystems with two external leads are considered, one has to ensure impedance matching at each interface. For the non-driven case we saw from impedance matching arguments that the optimal value of coupling was \( c = 1 \). Now the external lead is coupled to the filter. But we can generalize the idea of the non-filtered system by choosing the lead-filter coupling such that \( \Gamma = c J_f \), with \( c = 1 \). However now we have to consider how the system and leads are coupled. Since the two subsystems have different lattices the choice of coupling scheme is not straightforward. One choice is to imagine that that the last column of the filter couples to the first column of the system. Another is to imagine that the filter couples to several columns in the system. In that case it is natural to assume that the last column of the filter couples to several columns in the system. This is a simple one band model which is exactly what an ideal energy filter has. The Hamiltonian for the filter is

\[
H_{\text{filter}} = J_f \sum_{\langle ij \rangle} \left( c_i^\dagger c_j + \text{h.c.} \right) \tag{6.2.2}
\]

where \( J_f \) is the nearest neighbor hopping parameter. The spectrum of this model is given by

\[
E(k_x, k_y) = 2J_f \left( \cos(k_x a) + \cos(k_y a) \right) \tag{6.2.3}
\]

where \( a \) is the lattice constant of the 2D square lattice. The bandwidth of this system is given by \( 8J_f \).

In order for the filter to work this bandwidth needs to be small compared to the driving frequency. The band of this model is centered around \( E = 0 \). This is good for checking the \( E = 0 \) gap but won’t allow us to check the \( E = \frac{\hbar \Omega}{2} \) gap. We wish to probe both gaps. Therefore we add an offset term to the system of the form \( -V_g I \). Here \( I \) denotes the identity matrix of the same dimension as the physical dimension of the driven system and \( V_g \) is a gate voltage. We choose this name for the parameter since a natural way to implement such a term is to put a gate underneath the driven system that can be used to control the position of the systems energy levels by tuning the gate voltage. In this way we can keep the 2 filters fixed and probe the time-averaged differential conductance in different gaps by sweeping over the gate voltage. The full system Hamiltonian then reads

\[
H(t) = J_f \sum_{\langle ij \rangle \in \text{filter}_1} \left( c_i^\dagger c_j + \text{h.c.} \right) + \sum_{\langle ij \rangle \in \text{system}} \left( J_{ij}(t) c_i^\dagger c_j + \text{h.c.} \right) - V_g \sum_{i \in \text{system}} c_i^\dagger c_i + J_f \sum_{\langle ij \rangle \in \text{filter}_2} \left( c_i^\dagger c_j + \text{h.c.} \right). \tag{6.2.4}
\]

The computation of retarded Floquet Green’s functions for this system are done with a slight modification. Now the retarded Floquet Green’s functions are computed at a fixed energy, but are functions of gate voltage \( G^{r(n)}(E, V_g) \). The energy has been fixed at \( E = 0 \) for all computations. When computing differential conductances this correspond to putting the external chemical potential \( \mu = 0 \).

Now that 3 subsystems with two external leads are considered, one has to ensure impedance matching at each interface. For the non-driven case we saw from impedance matching arguments that the optimal value of coupling was \( c = 1 \). Now the external lead is coupled to the filter. But we can generalize the idea of the non-filtered system by choosing the lead-filter coupling such that \( \Gamma = c J_f \), with \( c = 1 \). However now we have to consider how the system and leads are coupled. Since the two subsystems have different lattices the choice of coupling scheme is not straightforward. One choice is to imagine that that the last column of the filter couples to the first column of the system. Another is to imagine that the filter couples to several columns in the system. In that case it is natural to assume that the last column of the filter couples to several columns in the system. This is a simple one band model which is exactly what an ideal energy filter has.
couples to the second column in the system and that the second last column of the filter couples to the first column of the system. We choose the first option. In addition to the choice of coupling scheme we must also choose the value of coupling carefully. We previously chose the system-lead coupling based on the hopping parameters in the system. Since the system and filters have the different hopping parameters \( J_f, J_1 \) we need to choose the system filter coupling in terms of these. A natural choice is just to choose the system filter coupling as the average of the two couplings \( J_{sf} = \frac{J_1 + J_f}{2} \). The is the choice we stick to here.

\[
J_{sf} = \frac{J_1 + J_f}{2}
\]

We now present results for the time-averaged differential conductance using energy filtered leads. For the simulations we have chosen a system of size \( L = 50, W = 81 \). The filters used have dimensions \( L_f = 100 \) and also \( W_f = 81 \). The truncation parameter is \( M = 3 \). The system and drive parameters are \( J_1 = 1, \Omega = 3 \) and \( \lambda = 0.5 \). We have used the gate voltage to sweep the gap at \( E = 0 \) and the gap at \( E = \frac{\Omega}{2} \). These results are depicted in Figs. 6.6a and 6.6b. We see that unlike the unfiltered case we actually recover almost perfectly quantized time-averaged differential conductance as one would have hoped. The improvement is especially good in the gap at \( E = \frac{\Omega}{2} \) where the values lie around \( \approx 1 \) without the filter. Instead with the filter we almost get the quantized value of \( 2e^2/h \) as expected since there are two edge modes in this gap. We are still trying to find out how to get completely flat plateaus. In Appendix C.3 we present similar results but for shorter filter lengths. There the results are not as good and we speculate that the deviation is due to finite size effects of the filter.

### 6.2.1 Particle- and current densities of the energy filtered graphene model

We will now focus on the spatial aspects of transport through the driven filtered system. If the filter works as intended the transport should be mediated by the edge states alone. In section 4.4.2 we found an expression for the time-averaged particle and current densities in the steady state. The formulas we derived for the densities involves an energy integral. These formulas yields the time-averaged densities by integrating up contributions from all states below the chemical potential of the two leads. This also involves all the bulk states at those energies. However we are only interested in the population of states due to the excess chemical potential on the left side. Therefore instead of computing the time-averaged particle density, we compute the difference in time-averaged particle density between two different steady states. The first steady state will be the one where the chemical potential of the two leads are the same. The second configuration is the one where the chemical potential of the left lead is shifted by a small amount \( eV \) compared to the right lead. This is the configuration we have used to calculate the time-averaged differential conductance. The difference between the time-averaged particle density of the two steady states will therefore tell us which additional states are populated at a given energy by raising the chemical potential by a small amount on the left side. The difference in between steady states is given

![Figure 6.6: a) Time-averaged differential con in the region around the \( E = 0 \) gap for a transport setup without filter and one with a filter. b) Non-equilibrium distribution function in the region around the \( E = \frac{\Omega}{2} \) gap for a transport setup without filter and one with a filter.](image-url)
by:
\[ \Delta \langle n_i(t) \rangle \equiv \frac{\langle n_i(t) \rangle_{\mu_1=\mu_2+eV} - \langle n_i(t) \rangle_{\mu_1=\mu_2}}{eV} = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} \left( G^{r(n)}(\mathcal{E}) \Gamma_L \left( G^{r(n)}(\mathcal{E}) \right)^\dagger \right)_{i,i}. \]  

(6.2.5)

We use this formula to compute the difference in time-averaged particle density between the two steady states in two situations. In the first situation the chemical potentials both reside in the gap at \( E = 0 \) with \( \mu_2 = 0 \). In this second situation a gate voltage \( V_g = 1.5 \) is applied to the system such that the chemical potentials are both inside the middle of gap at \( E = \frac{\Omega}{2} \) with \( \mu_2 = 0 \). Once more we consider systems of size \( L = 50 \) and 81 and the system parameters used are \( J_1, \Omega = 3 \) and \( \lambda = 0.5 \). The filters used have the parameters \( J_f = 0.25, L_f = 50 \) and \( W_f = 81 \). That is we have used the same parameters as we did to find time-averaged conductance in the on-resonant case. The results for both situations are depicted in Figs. 6.7a and 6.7b.

Figure 6.7: a) The picture shows the difference in particle density between the two steady states around at \( E = 0 \). b) A picture similar to that in Fig. 6.7a but for the laser induced gap at \( E = 1.5 \). System, filter and drive parameters are the same as in Fig. 6.7a.

We see that the additional particles injected from the left lead only occupy states along the left and right edge in Fig. 6.7a and Fig. 6.7b respectively. This indicate that these current arising from these particles are carried by edge states. In addition we see that particles are sucked into the right filter almost immediately after arriving at the system filter boundary. The considerations for the particle density are also true for the time-averaged current density which also involves an integral over energy. By the same argument we are only interested in the excess current that appear due to a finite bias. Here we also only expect local currents to appear in the region around the edges.

\[ \Delta \langle j_{ij}(t) \rangle \equiv \frac{\langle j_{ij}(t) \rangle_{\mu_1=\mu_2+eV} - \langle j_{ij}(t) \rangle_{\mu_1=\mu_2}}{V} = \frac{2e^2}{h} \sum_{m,n=-\infty}^{\infty} \text{Im} \left[ \left( G^{r(n)}(\mathcal{E}) \Gamma_L \left( G^{r(m)}(\mathcal{E}) \right)^\dagger \right)_{ij} J_{\rho(m-n)}(\lambda) e^{i\rho(m-n)(\pi-\phi_{ij})} \right]. \]  

(6.2.6)
To understand the direction of the current between different bonds we have applied the following color coded sign convention. The convention is seen in Fig. 6.8. We have obtained the current densities for the graphene system. The parameters used are the same used for the particle densities: \( J_1 = 1, \Omega = 3, \lambda = 0.5, L = 50, W = 81, L_f = 50, W_f = 81 \). We see that the only additional current injected from the left lead runs along the edges in both cases. Furthermore we computed the values of the horizontal current which are indicated by the black vertical lines on Figs. 6.9a and 6.10a. The value of the current density of those horizontal lines \( j_x \) are depicted in Fig. 6.9b and 6.10b. In both cases they are in good agreement with the results we found in section 6.2 (see figure legends).

Figure 6.9: a) Figure of the difference in current density between the two steady states. The chemical potentials are both zero such that the \( E = 0 \) gap is probed b) Plot of the value of current density of the horizontal bonds in Fig. 6.9a indicated by the black vertical line.
Figure 6.10: a) Figure of the difference in current density between the two steady states. The chemical potential is 1.5 for the unfiltered system. The filtered system has $\mu = 0$ and $V_g$ such that the $E = \frac{1}{2}$ gap is probed b) Plot of the value of current density of the horizontal bonds in Fig. 6.10a indicated by the black vertical line.

6.3 Non-equilibrium distribution functions for the graphene model

The study of the non-equilibrium distribution functions in Floquet topological insulators is an open area of research. The idea of tailoring external fermionic and bosonic baths to create an ideal insulator like steady state has already been explored in several papers [13, 15]. Here we obtain non-equilibrium distributions using Floquet Green’s functions. In section 4.4.3 a formula for the non-equilibrium distribution function of a periodically driven system in a two terminal setup was derived. We will now apply Eqs. (4.4.18), (4.4.3) and (4.4.22) to compute the non-equilibrium distribution function in two cases. First we would like to find the non-equilibrium distribution function for the graphene model without any energy filtered leads, like in section 6.1. We focus on the steady state where the chemical potential in the two leads are the same. The analysis can also be done with a small bias difference, but for now we are only interested in how different external baths leads to different steady states. Since no energy filtered lead is used what the steady state distribution function should look like. We will then compare this non-equilibrium distribution function to one obtained for the two terminal setup used in section 6.2 where energy filtered leads are present. The system and drive parameters should be the same such that the only difference is the addition of energy leads. The results will then tell us how well our model for the energy filtered lead works.
Figure 6.11: a) Non-equilibrium distribution functions with chemical potentials $\mu = 0$. The blue data points indicate the values of the distribution without an energy filtered lead and the orange data points indicate the values of the distribution with an energy filtered lead. b) Non-equilibrium distribution functions probing the gap at $E = \frac{\Omega}{2}$. The blue data points indicate the values of the distribution without an energy filtered lead with chemical potentials $\mu = 0$. The orange data points indicate the values of the distribution with an energy filtered lead, using $\mu = 0$ and $V_g = 1.5$.

We have found and compared distribution functions in to different cases. In the first case the distribution function is found without energy filtered leads, with $\mu = 0$ for both leads. This is compared to the case where energy filtered leads are used, for which we also put $\mu = 0$ and fix $V_g = 0$ such that we compare the two distributions around the $E = 0$ gap. The parameters used without filter are $J_1 = 1$, $\Omega = 3$, $\lambda = 0.5$. These parameters are the same for the setup with the filter. The filters used have the hopping parameter $J_f = 0.25$. The two distribution functions are depicted in Fig. 6.11a. We see that in both gaps the energy filtered lead yields a steady state which looks identical to the Fermi-Dirac distribution of equilibrium systems. Without the filter however the edge states in the gap are not fully populated.

In addition we would also like to check the distribution function in the case where the chemical potentials are fixed in the $E = \frac{\Omega}{2}$ gap. For the setup with wide band leads we therefore choose $\mu = 1.5$. The system and drive parameters used are the same as before. For the filtered system we instead choose $\mu = 0$ and $V_g = 1.5$. This choice reflects the fact that the filter is centered around $E = 0$. Therefore to probe the same region in the driven system we instead shift the energies of the driven system by applying a gate voltage such that the laser induced gap is centered at $E = 0$. Here the system and drive parameters are identical to those of the non-filtered case. The filters used once again have the hopping parameter $J_f = 0.25$. These to distribution functions are compared in Fig. 6.11b. In the $E = \frac{\Omega}{2}$ gap the occupation in the steady state without a filter below the chemical potential seems to be even lower compared to distribution function for the $E = 0$ gap. Despite the fact that the filters seems to produce the best scenario possible in both cases, it is natural to ask why it works so well? Here we only consider non-interacting systems. That means that there are in fact no relaxation mechanisms present. Except for the Pauli exclusion principle which forbids electrons from occupying the same states and therefore has a level repelling effect. In reality effects such as: impurities, phonons, electron-electron interactions and electron-photon interactions have to be taken into account to get a more realistic model for the steady states of Floquet topological insulators. The results here indicate that the filter does what it was designed to do, in the non-interacting case.

6.4 Discussion

While the model introduced for the filter had the advantage of conceptual simplicity it is not realistic to find a material described by this single band model. In reality however we might imagine that such a single narrow band does exists within some larger bandstructure. In that case a single band might still act as an energy filtering lead if it is well separated from the other bands in the host material. In this case the driving frequency has to be compared to not only the bandwidth of the filter but also the
interband-width of the material that contain the narrow band. Such a material might still work well as a filter if one only consider one or two-photon resonances. A promising candidate material could be highly mismatched alloys featuring narrow bands, which has recently been realized in solar-cells [13, 48]. Another candidate for narrow bands could be impurity bands inside of materials with a wide band gap. Such impurity bands form naturally when enough impurities are present in a material sample [20].

The strategy of using energy filtered leads can also be applied to other types of periodically driven systems where photon assisted tunneling is present. These processes are also a problem in other periodically driven topological systems such as Floquet-Majorana wires which was recently proposed [10]. These systems are an example of so called topological superconductors that like insulators have topological properties associated with their quasiparticle spectrum. A characteristic signature of these systems is a peak at zero bias in the differential conductance. If present such a peak hints toward the existence of Majorana fermions. This possibility have already been studied by many different people for non-driven Majorana systems. For periodically driven Floquet-Majorana wires it was pointed out that such a quantization is absent due to a sum rule like the one we discussed previously in this chapter [45]. However by the same argument applied here an energy filtered lead could also be used in such systems to restore quantization of the differential conductance. Floquet-Majorana wires were originally proposed for ultra cold atom platforms. A group has recently shown that it is possible to create artificial contacts and carry out transport experiments in such systems. Due to the amazing control in such systems one could imagine that a one dimensional version of the ideal one band model presented in Eq. (6.2.2) could be made artificially using atoms. If possible the strategy presented here would also be applicable to the proposed Floquet-Majorana system.
Chapter 7

Conclusion and outlook

In this thesis quantum transport through periodically driven systems was explored. A formalism for periodically driven systems was first introduced. Subsequently topological insulators was introduced. The Chern insulator and its related physical properties where explained. An introduction to the recent work on generating non-equilibrium versions of these systems using periodic driving was given. It was argued that unlike their non-driven counterpart Floquet topological insulators do not generally exhibit quantized two terminal conductance. A simple picture was given to explain this deviation. Furthermore a recent proposal to restore conductance quantization in periodically driven topological insulators by replacing wide band leads with energy filtering narrow band leads, was briefly introduced.

To deal with periodically driven systems in a transport setting a formalism for non-equilibrium Green’s functions was introduced. This formalism was used to obtain a number of different quantities. A result obtained in many recent papers for the steady state current was re-derived using the Jauho-Wingreen-Meir formula. For the steady states of periodically driven systems it was shown how to obtain time-averaged differential conductance, time-averaged local density of states, time averaged particle- and current density as well as non-equilibrium distribution functions. The Recursive Green’s function technique for non-equilibrium Green’s functions was introduced and explained. This technique was then applied for numerical computations to prevent the issue of large computation times.

Finally the formalism developed in the early chapters of the thesis was used to put the recent proposal of energy filtered leads to a test. By comparing results for the time-averaged differential conductance of filtered and non-filtered steady states of periodically driven systems we showed that energy filtered leads effectively restores quantization by having only one edge state sideband mediate the transport. Several other quantities was obtained for the steady state of the driven system. Our results for the particle- and current density also concluded that transport inside the gap was mediated by edge states alone. Furthermore we found the non-equilibrium distribution function of the steady state at zero bias with and without energy filtered leads. The results showed that filters produced non-equilibrium distributions functions similar to the Fermi-Dirac distribution of equilibrium fermionic systems.

Although the results presented here are promising there are still many aspects of transport through Floquet topological insulators which needs to be explored. First we have to explore how the time-averaged differential conductance depends on the filter size. If what we see are really finite size effects it should be possible to get a more clear plateau by using larger filters. In addition we would like to investigate the non-equilibrium distribution function further. Specifically we would like to find non-equilibrium distribution functions for the edge regions alone. For sufficiently large system length the region away from the corners of the 2D system will be translationally invariant along the edge. Therefore it would be interesting to see if we could get a momentum resolved distribution function for the edge states. More generally there are several interesting directions in the field of Floquet topological insulators which hopefully will be explored in the years to come. Here some of the promising directions are briefly reviewed.

All results given in this thesis was for non-interacting systems. Interactions are of particular importance in periodically driven systems, since they lead to heating. This has a dramatic effect on the non-equilibrium distribution function of Floquet topological insulators. This problem has already been addressed by many different people. Some have argued that special tailored baths such as the energy
filtered leads can be used to control the steady state of periodically driven systems. One example is the energy filtered leads that have been the focus of this thesis. But also baths with bosonic degrees of freedom, such as phonon baths have been proposed as a cooling mechanism for interacting periodically driven systems. While electron-electron interactions generally lead to heating, electron-phonon interactions can be useful since the heat can be dumped into the phonon bath. How different interactions compete and what different type of steady states that can be created is on-going research [51, 52].

Other people have suggested looking into transient regimes of transport. When interactions are included it is not given that a periodically driven systems assumes a nice steady state in the first place. Therefore studying the transient regime yields further insight into the interplay between periodic driving and interactions. In some cases it is possible to have transients that are very long lived, so called prethermal states. Recently it has been shown that such transients may in fact display universal behavior [19].

Finally it has been proposed that heating could be prevented by considering strongly disordered Floquet topological insulators. Specifically a lot of attention has been devoted to the study of so called many-body localized (MBL) systems. These are of huge interest, not just within the field of periodically driven systems, but quantum many-body systems in general. It has been proposed that if MBL is present in periodically driven systems it would prevent the system from heating up [53]. The system will still be periodic in time, but it won’t be able to absorb energy from the external drive. In a Floquet topological insulator MBL could be used as a tool to control the steady state of such systems, even in the presence of interactions [54]. While strong disorder usually ruins topological phases, a new type of Floquet topological insulator has recently been found. Here the interplay between periodic driving and MBL leads to a topological phase with no counterpart in equilibrium [12].

In addition to the theoretical progress within the field, it will also be interesting to see what experimental discoveries that will be made in the years to come.
Bibliography


Appendices
Appendix A

Derivations for Chapter 3

A.1 Bulk Hamiltonian

In order to obtain a Hamiltonian for the bulk we perform a change of basis by a Fourier transform. First some comment on counting. The sum runs over all sites \( i \), while the \( j \) labels the 3 nearest neighbors. To avoid double counting it is useful to distinguish between sites on the \( A \) and \( B \) sublattice. Therefore we use the convention that the sites \( i \) that are summed over are only those on the \( A \) sublattice and that the neighboring sites \( j \) are those on the \( B \) sublattice. The Fourier transform of the creation and annihilation operators may then be written as

\[
c_i = \frac{1}{\sqrt{N}} \sum_k e^{i k \cdot r_i} c_{kA} \quad c_j = \frac{1}{\sqrt{N}} \sum_k e^{i k \cdot (r_i + r_j)} c_{kB}
\]  

(A.1.1)

Here \( k \) is the crystal momentum, \( A \) and \( B \) are the sublattice indices, and \( N \) serves as a normalization factor and denotes the number of sites on one sublattice. The nearest neighbor Hamiltonian can now be written as

\[
H_{NN} = \frac{J_1}{N} \sum_{(ij), k, k'} c_{k', A} c_{k, B} e^{i k \cdot (r_i + r_j)} e^{-i k' \cdot r_i} + \text{h.c.}
\]

(A.1.2)

We now introduce the shorthand notation

\[
H_{NN} = \sum_k c_{kA} \mathcal{H}(k) c_{kB}. \quad \text{With} \quad J(k) = J_1(\exp^{i k \cdot \delta_1} + \exp^{i k \cdot \delta_2} + \exp^{i k \cdot \delta_3}) + \text{h.c.}
\]  

(A.1.3)

In the \( c_{kA}, c_{kB} \) basis the Hamiltonian takes the form:

\[
H = \sum_k c_k^\dagger \mathcal{H}(k) c_k,
\]  

(A.1.4)

where we defined

\[
\mathcal{H}(k) = \begin{pmatrix} 0 & J(k) \end{pmatrix} \begin{pmatrix} J(k)^* & 0 \end{pmatrix} \quad c_k = \begin{pmatrix} c_{kA} \\ c_{kB} \end{pmatrix} \quad c_k^\dagger = \begin{pmatrix} c_{kA}^\dagger \\ c_{kB}^\dagger \end{pmatrix}.
\]  

(A.1.5)

We would like the Hamiltonian to satisfy Bloch’s theorem, that is \( \mathcal{H}(k + G) = \mathcal{H}(k) \). Here the vector \( G \) represents a translation in momentum space which is generally written in terms of the reciprocal lattice vectors

\[
b_1 = \frac{2\pi}{3\alpha} (1, \sqrt{3}) \quad b_2 = \frac{2\pi}{3\alpha} (1, -\sqrt{3})
\]  

(A.1.6)
These can be determined from the relation $b_i \cdot a_j = 2\pi \delta_{ij}$. Since the lattice has translational invariance with respect to the vectors $a_1$ and $a_2$ we need to get rid of the nearest neighbor vectors. In order to do so we now make a gauge-transformation in order to remove the factor containing $\delta$ so we make a gauge-transformation in order to remove the factor containing $\delta$.

$$\delta_{\bf k, A} \rightarrow \delta_{\bf k, A} e^{-i\bf{k} \cdot \delta} \quad J(\bf{k}) \rightarrow J(\bf{k}) = J_1(1 + e^{i\bf{k} \cdot a_1} + e^{i\bf{k} \cdot a_2})$$ (A.1.7)

Diagonalizing the on-site potential term is similar to the nearest neighbor term accept that it doesn’t involve hopping between sublattices. We would however still like to use the $A$ and $B$ sublattice convention. Therefore we write the on-site potential term as

$$H_M = \sum_{\alpha} \sum_i M_{\alpha} e^{i\phi_{i,A}} c_{i,\alpha}$$ (A.1.8)

where the sum over $i$ runs over unit cells and the parameter $M_{\alpha}$ is defined as

$$M_{\alpha} = \begin{cases} M & \text{if } \alpha \in \text{Sublattice A} \\ -M & \text{if } \alpha \in \text{Sublattice B} \end{cases}.$$ (A.1.9)

The Fourier transform may then be written as

$$H_M = \sum_{\alpha} \sum_i M_{\alpha} c_{i,\alpha}^\dagger c_{i,\alpha} = \sum_{\alpha} \sum_k \sum_{k'} \delta_{\bf{k,k'}} M_{\alpha} e^{i\phi_{k,\alpha}} c_{k,\alpha} = \sum_{\alpha} \sum_k M \left( c_{k,\alpha}^\dagger c_{k,\alpha} - c_{k,\beta}^\dagger c_{k,\beta} \right).$$ (A.1.10)

If we use the vectors defined in Eq. (A.1.5) we may write $H_M$ as

$$H_M = M \sum_k e^{i\phi_{k,\alpha}} c_{k,\alpha}.$$ (A.1.11)

The term containing the second nearest neighbors can be diagonalized in the same fashion as for nearest neighbor hopping. However there is 6 nearest neighbors with different signs on $\phi$. The sign convention is such that

$$\text{A sublattice : } v_{il} = \begin{cases} 1 & \text{if } l = 1, 3, 5 \\ -1 & \text{if } l = 2, 4, 6 \end{cases} \quad \text{B sublattice : } v_{il} = \begin{cases} -1 & \text{if } l = 1, 3, 5 \\ 1 & \text{if } l = 2, 4, 6 \end{cases}$$ (A.1.12)

We start by performing a Fourier transform for the sites on the A sublattice. The Fourier transform becomes:

$$H_{\text{NNN},A} = \sum_{k} c_{k,\alpha}^\dagger c_{k,\alpha} \left( e^{-i\bf{k} \cdot r_1 + i\phi_{v_1}} + e^{-i\bf{k} \cdot r_2 + i\phi_{v_2}} + e^{-i\bf{k} \cdot r_3 + i\phi_{v_3}} + e^{-i\bf{k} \cdot r_4 + i\phi_{v_4}} + e^{-i\bf{k} \cdot r_5 + i\phi_{v_5}} + e^{-i\bf{k} \cdot r_6 + i\phi_{v_6}} \right)$$

By writing out the $l$ sum we get

$$H_{\text{NNN},A} = J_2 \sum_k c_{k,\alpha}^\dagger c_{k,\alpha} \left( e^{-i\bf{k} \cdot r_1 + i\phi} + e^{i\bf{k} \cdot r_1 + i\phi} + e^{-i\bf{k} \cdot r_2 + i\phi} + e^{i\bf{k} \cdot r_2 + i\phi} + e^{-i\bf{k} \cdot r_3 + i\phi} + e^{i\bf{k} \cdot r_3 + i\phi} \right)$$

We now use that $r_1 = -r_4, r_2 = -r_5, r_3 = -r_6$. To write the Hamiltonian above as

$$H_{\text{NNN},A} = J_2 \sum_k c_{k,\alpha}^\dagger c_{k,\alpha} \left( e^{i\bf{k} \cdot r_1 + i\phi} + e^{i\bf{k} \cdot r_2 + i\phi} + e^{i\bf{k} \cdot r_3 + i\phi} \right)$$

Using $r_1 = a_1, r_2 = a_2, r_3 = a_1 - a_2$ we can write the Hamiltonian for the $A$ sublattice as

$$H_{\text{NNN},A} = J_2 \sum_k c_{k,\alpha}^\dagger c_{k,\alpha} \left( \cos(k \cdot a_1 + \phi) + \cos(k \cdot a_2 + \phi) + \cos(k \cdot (a_2 - a_1) + \phi) \right)$$

$$= 2J_2 \sum_k c_{k,\alpha}^\dagger c_{k,\alpha} \left( \cos(k \cdot a_1) \cos(\phi) + \cos(k \cdot a_2) \cos(\phi) + \cos(k \cdot (a_2 - a_1)) \cos(\phi) + \sin(k \cdot a_1) \sin(\phi) - \sin(k \cdot a_2) \sin(\phi) - \sin(k \cdot (a_2 - a_1)) \sin(\phi) \right)$$ (A.1.13)
In the $c_{k_A}, c_{k_B}$ basis these terms enter the first diagonal entry of the Hamiltonian. The calculation for the $B$-sublattice is completely similar except for the fact that the sign convention $\nu_l$ is opposite. This effectively corresponds to $\phi \rightarrow -\phi$. This will only change the sign of the sine terms. This means that the cosine terms can be written as proportional to the identity operator while the sine terms can be written as proportional to $\sigma_z$. The next nearest neighbor term is therefore

\[ H_{\text{NNN}} = \sum_k c_k^\dagger \mathcal{H}(k) c_k, \quad \mathcal{H}(k) = \begin{pmatrix} \epsilon(k) + \Delta(k) & 0 \\ 0 & \epsilon(k) - \Delta(k) \end{pmatrix}, \]  

(A.1.14)

where we defined

\[ \epsilon(k) = 2J_2 \cos(\phi) \left( \cos(k \cdot a_1) + \cos(k \cdot a_2) + \cos(k \cdot (a_2 - a_1)) \right) \]

\[ \Delta(k) = -2J_2 \sin(\phi) \left( \sin(k \cdot a_1) + \sin(k \cdot a_2) + \sin(k \cdot (a_2 - a_1)) \right). \]  

(A.1.15)

The full Hamiltonian can now be written in the form

\[ H = \sum_k c_k^\dagger \mathcal{H}(k) c_k, \]  

(A.1.16)

where we defined the operators:

\[ c_k = (c_{k_A}, c_{k_B})^T, \quad c_k^\dagger = (c_{k_A}^\dagger, c_{k_B}^\dagger), \]  

(A.1.17)

and the bulk Hamiltonian

\[ \mathcal{H}(k) = \epsilon(k) I + d(k) \cdot \sigma, \]  

(A.1.18)

Here $I$ denotes the $2 \times 2$ identity matrix and $\sigma$ is a vector containing the Pauli matrices. The quantities $\epsilon(k)$ and $d(k)$ are given by

\[ d_1(k) = \text{Re} (J(k)) \quad , \quad d_2(k) = \text{Im} (J(k)) \quad , \quad d_3(k) = \Delta(k) \]  

(A.1.19)

By inspecting Eqs. (A.1.7), (A.1.11) and (A.1.15) we see that the quantities for the Haldane model are given by:

\[ \epsilon(k) = 2t_2 \cos(\phi)(\cos(k \cdot a_1) + \cos(k \cdot a_2) + \cos(k \cdot (a_2 - a_1)) \]

\[ d_1(k) = 1 + \cos(k \cdot a_1) + \cos(k \cdot a_2) \]  

(A.1.20)

\[ d_2(k) = \sin(k \cdot a_1) + \sin(k \cdot a_2) \quad , \quad d_3(k) = M + t_2 \sin(\phi)(\sin(k \cdot a_1) - \sin(k \cdot a_2) - \sin(k \cdot (a_1 - a_2)) \]  

(A.1.21)

### A.2 Formula for the Chern number of a 2 band Continuum Hamiltonian

Consider the continuum Hamiltonian for a generic 2 band model

\[ \mathcal{H}(k) = k_x A_{1b} \sigma_b + m \sigma_3 \]  

(A.2.1)

Where $a$ and $b$ are dummy indices with $a, b = 1, 2$ and $\sigma$ denotes the Pauli matrices. This Hamiltonian describes only one valley. However it can be either one so at the end of the calculation we can just add up contributions for other valleys. The Berry curvature for a single valley in the valence band can be written as [22]

\[ B_n = \frac{1}{2d^2} m \text{Det}(A) \]  

(A.2.2)

With $d = \sqrt{E_m k_i A_{ij} A_{mj} + m^2}$. The Chern number of the valence band can then be calculated as

\[ C = \frac{1}{2\pi} \int \int B_n d^2 k = \frac{1}{2\pi} \frac{m \text{Det}(A)}{2} \int \frac{1}{(k_n k_i A_{ij} A_{mj} + m^2)^2} (d^2 k) \]  

(A.2.3)

We now introduce the polar coordinates $k_x = k \cos(\theta)$ and $k_y = k \sin(\theta)$, where $k = \sqrt{k_x^2 + k_y^2}$. The Chern number of the valence band can be written as

\[ C = \frac{1}{2\pi} \frac{m \text{Det}(A)}{2} \int_0^{2\pi} d\theta \int \frac{k}{\sqrt{D(\theta)k^2 + m^2}} dk \]  

(A.2.4)
With \( D(\theta) = \cos^2(\theta)A_{1j}A_{1j} + \sin^2(\theta)A_{2j}A_{2j} + 2\cos(\theta)\sin(\theta)A_{1j}A_{2j} \). This integral can be solved by substitution \( x = D(\theta)k^2 \), \( dk = dx/2D(\theta)^{1/2} \). The integral then becomes

\[
\mathcal{C} = \frac{1}{8\pi} m \text{Det}(A) \int_0^{2\pi} \frac{1}{D(\theta)} d\theta \int_0^\infty \frac{1}{\sqrt{x + m^2}} dx
\]

(A.2.5)

The theta integral is computed using the identity

\[
\int_0^{2\pi} \frac{1}{\cos^2(\theta)A_{1j}A_{1j} + \sin^2(\theta)A_{2j}A_{2j} + 2\cos(\theta)\sin(\theta)A_{1j}A_{2j}} d\theta = \frac{2\pi}{|\text{Det}(A)|}
\]

(A.2.6)

The \( x \) integral is computed by using \( s = x + m^2 \)

\[
\int_0^\infty \frac{1}{\sqrt{s} + m^2} ds = \int_{s(0)}^{s(\infty)} \frac{1}{\sqrt{s}} ds = \frac{-2}{\sqrt{3}} s(0) = \frac{2}{\sqrt{m^2}} = \frac{2}{|m|}
\]

(A.2.7)

Putting this together we obtain a formula for the Chern number of the valence band

\[
\mathcal{C} = \frac{\text{sign}(m)\text{sign}(\text{Det}(A))}{2}
\]

(A.2.8)

For the valley Hamiltonians in the main text we have: \( \text{Det}(A) = +1 \) and \( m = 3\sqrt{3}J_2 \sin(\phi) - M \) for the Hamiltonian in valley \( K \) and \( \text{Det}(A) = -1 \) and \( m = -3\sqrt{3}J_2 \sin(\phi) - M \) for the Hamiltonian in valley \( K' \). Therefore the Chern number becomes

\[
\mathcal{C} = \left( \frac{\text{sign}(3\sqrt{3}J_2 \sin(\phi) - M)}{2} - \text{sign}(M - 3\sqrt{3}J_2 \sin(\phi)) \right).
\]

(A.2.9)

The sum of Chern numbers of the two bands has to be zero as stated in the main text. Therefore the Chern number of the conduction band will simply be minus that of the Chern number of the valence band.

### A.3 The Haldane Hamiltonian in a ribbon geometry

In order to see edge states we need to study the Haldane model in a finite geometry. To do so we consider a ribbon graphene sheet with zig-zag edges. That is a sheet which has a finite width but is infinitely long such that periodic boundary conditions are still valid in one direction. This is equivalent to a having graphene sheet wrapped onto a cylinder. For a system in the ribbon geometry it is useful to define Fourier transforms of the creation and annihilation operators where the transform is performed with respect to the direction containing translational invariance. Here we choose this direction to be the \( y \)-direction. But before doing so we first rewrite the Haldane Hamiltonian using a new labeling convention. Since the new unit cell is a whole strip it is useful to label each operator by its strip index as well as a site index that describes the site on the strip in question. Using the new labeling convention the nearest neighbor term in the Haldane Hamiltonian reads:

\[
H_{nn} = J_1 \sum_{j=1}^{\frac{L}{2}} \sum_{n=-\infty}^{\infty} (c_{2j-1,n}^\dagger c_{2j,n} + \text{h.c.}) + J_1 \sum_{j=1}^{\frac{L}{2}} \sum_{n=-\infty}^{\infty} (c_{2j-1,n}^\dagger c_{2j,n-1} + \text{h.c.})
\]

\[
+ J_1 \sum_{j=1}^{\frac{L}{2}-1} \sum_{n=-\infty}^{\infty} (c_{2j,n}^\dagger c_{2j+1,n} + \text{h.c.})
\]

(A.3.1)

The Semenoff term just adds an onsite potential so for the new unit cell this term reads:

\[
H_{\text{Semenoff}} = M \sum_{j=1}^{L} \sum_{n=-\infty}^{\infty} (c_{2j-1,n}^\dagger c_{2j-1,n} - c_{2j,n}^\dagger c_{2j,n})
\]

(A.3.2)
The Haldane term can be written for the ribbon geometry in the same way as the nearest neighbor:

\[
H_{\text{Haldane}} = J_2 \sum_{j=1}^L \sum_{n=-\infty}^{\infty} \left( e^{-i\phi} c_{2j-1,n}^\dagger c_{2j+1,n} + e^{i\phi} c_{2j,n}^\dagger c_{2j+2,n} + \text{h.c.} \right) \\
+ J_2 \sum_{j}^{L/2} \sum_{n=-\infty}^{\infty} \left( e^{-i\phi} c_{2j,n}^\dagger c_{2j,n+1} + e^{i\phi} c_{2j,n} c_{2j,n-1} + e^{i\phi} c_{2j-1,n}^\dagger c_{2j-1,n+1} + e^{-i\phi} c_{2j-1,n}^\dagger c_{2j-1,n-1} \right). 
\]  
(A.3.3)

We now define the Fourier transformed operators:

\[
c_{j,k_y} = \frac{1}{\sqrt{N}} \sum_{n=-\infty}^{\infty} c_{j,n} e^{-i k_y r_{j,n}}, 
\]  
(A.3.4)

\[
c_{j,k_y}^\dagger = \frac{1}{\sqrt{N}} \sum_{n=-\infty}^{\infty} c_{j,n}^\dagger e^{i k_y r_{j,n}}.
\]  
(A.3.5)

The Haldane Hamiltonian for a strip is then given by:

\[
H = J_1 \sum_{k_y} \sum_{j=1}^{L/2} \left( c_{2j,k_y}^\dagger c_{2j-1,k_y} \left( e^{i k_y \delta_1} + e^{i k_y \delta_2} + \text{h.c.} \right) + J_1 \sum_{k_y} \sum_{j=1}^{L/2-1} \left( c_{2j,k_y}^\dagger c_{2j+1,k_y} + \text{h.c.} \right) \\
+ \sum_{k_y} \sum_{j=1}^{L/2} \left( c_{2j-1,k_y}^\dagger c_{2j-1,k_y} \left( M + J_2 \left( e^{i (k_y a_1 - a_2) + \phi} + e^{-i (k_y a_1 - a_2) + \phi} \right) \right) \\
- c_{2j,k_y}^\dagger c_{2j,k_y} \left( M - J_2 \left( e^{i (k_y a_1 - a_2) - \phi} + e^{-i (k_y a_1 - a_2) - \phi} \right) \right) \right) \\
+ J_2 \sum_{k_y} \sum_{j=1}^{L/2-2} \left( c_{2j,k_y}^\dagger c_{2j+1,k_y} \left( e^{i (k_y a_1 + \phi)} + e^{i (k_y a_2 - \phi)} \right) + \text{h.c.} \right) \\
+ J_2 \sum_{k_y} \sum_{j=1}^{L/2-2} \left( c_{2j-1,k_y}^\dagger c_{2j+1,k_y} \left( e^{i (k_y a_1 - \phi)} + e^{i (k_y a_2 + \phi)} \right) + \text{h.c.} \right). 
\]  
(A.3.6)

This can be further simplified:

\[
H = 2J_1 \sum_{k_y} \sum_{j=1}^{L/2} \left( c_{2j,k_y}^\dagger c_{2j-1,k_y} \cos \left( \frac{\sqrt{3}}{2} k_y \right) + \text{h.c.} \right) + J_1 \sum_{k_y} \sum_{j=1}^{L/2-1} \left( c_{2j,k_y}^\dagger c_{2j+1,k_y} + \text{h.c.} \right) \\
+ \sum_{k_y} \sum_{j=1}^{L/2} \left( c_{2j-1,k_y}^\dagger c_{2j-1,k_y} \left( M + 2J_2 \cos \left( \sqrt{3} k_y + \phi \right) \right) - c_{2j,k_y}^\dagger c_{2j,k_y} \left( M - 2J_2 \cos \left( \sqrt{3} k_y - \phi \right) \right) \right) \\
+ 2J_2 \sum_{k_y} \sum_{j=1}^{L/2-2} \left( c_{2j,k_y}^\dagger c_{2j+1,k_y} \cos \left( \frac{\sqrt{3}}{2} k_y + \phi \right) + \text{h.c.} \right) \\
+ 2J_2 \sum_{k_y} \sum_{j=1}^{L/2-2} \left( c_{2j-1,k_y}^\dagger c_{2j+1,k_y} \cos \left( \frac{\sqrt{3}}{2} k_y - \phi \right) + \text{h.c.} \right). 
\]  
(A.3.7)

A.4 Analytic solution at the boundary between topological insulators

We start by defining the unitary transform

\[
U_y = e^{-i \frac{\pi}{6} \frac{y}{L}},
\]  
(A.4.1)
which corresponds to a $\frac{\pi}{2}$ rotation around the $y$-axis. When acting on Pauli matrices it has the following properties

\begin{align}
U_y \sigma_x U_y^\dagger &= -\sigma_z \\
U_y \sigma_y U_y^\dagger &= \sigma_y \\
U_y \sigma_z U_y^\dagger &= \sigma_x
\end{align}

(A.4.2)

We now make the unitary transform of the Hamiltonian and analyze it in the new basis:

\[ U_y H U_y^\dagger = -v_f \left( i\hbar \sigma_y \frac{\partial}{\partial x} - \hbar k_y \sigma_z \right) + m(x) \sigma_x \]

(A.4.3)

The solutions are spinors of the form:

\[ \Psi(x, y) = e^{-ik_y y} \begin{pmatrix} \phi_1(x) \\ \phi_2(x) \end{pmatrix} . \]

(A.4.4)

Plugging the spinor into the transformed Hamiltonian leads to the two equations:

\begin{align}
(E - \hbar v_f k_y) \phi_1(x) &= \left( m(x) + \hbar v_f \frac{\partial}{\partial x} \right) \phi_2(x), \\
(E + \hbar v_f k_y) \phi_2(x) &= \left( m(x) - \hbar v_f \frac{\partial}{\partial x} \right) \phi_1(x).
\end{align}

(A.4.5) (A.4.6)

We now look for solutions where $E = \pm \hbar v_f k_y$ like stated in the main text. Now the two solutions are decoupled and are simple differential equations. Their solutions are similar except for a difference in sign:

\[ \phi_{1/2}(x) = \mp \frac{1}{\sqrt{C}} e^{-\frac{1}{\sqrt{C}} \int_x^m(x')} . \]

(A.4.7)

Here we used the boundary condition, which is that $\phi_{1/2}(x)$ has to vanish at $x = \pm \infty$. Since these are wavefunctions they must be have norm unity, therefore the normalization constant $\frac{1}{\sqrt{C}}$ is included. The total solution may be written as

\[ \Psi(x, y) = \chi(x, y) \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix} , \quad \chi(x, y) = \frac{1}{\sqrt{C}} e^{ik_y y - \frac{1}{\sqrt{C}} \int_x^m(x')} . \]

(A.4.8)

### A.5 4x4 extended space matrix and dynamical gap opening

We will follow the analysis given in [27]. Here there is a different convention for the linearized Hamiltonian compared to the one used in this thesis. The Hamiltonians linear in momentum are rotated such that $\sigma_x \to \sigma_y$ and $\sigma_y \to -\sigma_x$. The results are of course equivalent since this merely correspond to a unitary transformation of the Hamiltonian. Here we follow the convention in [27]. There the Hamiltonian is

\[ H(t) = v_f \left( (k_x - A_x(t)) \sigma_x + (k_y - A_y(t)) \sigma_y \right) . \]

(A.5.1)

To derive the extendedspace Hamiltonian we start by finding the Fourier components of $H(t)$. The non-zero components $H_n$ are

\[ H_0 = \frac{1}{T} \int_0^T dt H(t) = v_f (k_x \sigma_x + k_y \sigma_y) = v_f (k_\pm \sigma_+ + k_- \sigma_-) , \]

(A.5.2)

where we defined $\sigma_\pm = \frac{\sigma_x \pm i \sigma_y}{2}$. The remaining components are

\[ H_1 = \frac{1}{T} \int_0^T dt H(t) e^{i\Omega t} = v_f eA_0 \frac{1}{T} \int_0^T dt \left( \cos(\Omega t) \sigma_x e^{i\Omega t} - \sin(\Omega t) \sigma_y e^{i\Omega t} \right) \\
= v_f eA_0 \frac{1}{2} (\sigma_x + \frac{1}{i} \sigma_y) = v_f eA_0 \sigma_-, \]

(A.5.3)
Once again we subtract the terms proportional to the identity on both sides and then subsequently take the square on both sides. We now subtract the terms proportional to the identity on both sides and write down the quasienergy of the 4 bands as:

The truncated extended space Hamiltonian then reads

In terms of Pauli matrices this may be rewritten as

We now go to the weak driving limit where

The eigenvalues are given by

We now define the parameters

and

We can now write down the quasienergy of the 4 bands as:

We now subtract the terms proportional to the identity on both sides and subsequently square both sides of the equality sign to get:

The eigenvalues are given by

where:

We now define the parameters

We can now write down the quasienergy of the 4 bands as:

We now go to the weak driving limit where \( \eta \ll 1 \). The \( \eta^4 \) term in \( \mu_\pm \) can then be ignored and we may write it as

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We now Taylor expand the inner square root, keeping only terms up to second order. Furthermore we now focus on the minus solution only:

\[ \mu_- \approx \sqrt{\left( 1 + \left( \frac{k}{k_0} \right)^2 + 2\eta^2 - 2 \frac{k}{k_0} \left( 1 + \frac{1}{2} \eta^2 \right) \right)} = \sqrt{(1 - \frac{k}{k_0})^2 + 2\eta^2 - \frac{k}{k_0} \eta^2} \]  

(A.5.14)

We are only interested in the spectrum in the region close to \( k = k_0 \) therefore we set \( \frac{k}{k_0} = 1 \) but keep the second order term

\[ \mu_- = \sqrt{(1 - \frac{k}{k_0})^2 + \eta^2} \]  

(A.5.15)

In the vicinity of \( k = k_0 \) the quasienergy bands of \( E_2 \) and \( E_4 \) becomes

\[ E_{2/4} = \frac{\hbar \Omega}{2} \left( 1 \pm \sqrt{(1 - \frac{k}{k_0})^2 + \eta^2} \right). \]  

(A.5.16)

This gap is located around \( \frac{\hbar \Omega}{2} \). The size of this gap between the bands at \( k = k_0 \) is then given by:

\[ \Delta_1 = \hbar \Omega \eta = ev_f A_0. \]  

(A.5.17)

### A.6 Driven graphene sheet in a ribbon geometry

We now investigate what happens to the graphene model when it is subject to circularly polarized light. We start from the Hamiltonian

\[ H(t) = \sum_{(ij)} J_i e^{iA_{ij}(t)} c_i^\dagger c_j + \text{h.c.}, \]  

(A.6.1)

where \( A_{ij}(t) = \frac{\hbar}{2} \mathbf{A}(t) \cdot (\mathbf{r}_j - \mathbf{r}_i) \) and the vector potential is given by \( \mathbf{A}(t) = A(\cos(\Omega t), \rho \sin(\Omega t)) \). Where \( \Omega \) is the driving frequency and \( A \) is the field strength. The parameter \( \rho \) indicates left/right polarization of the external light field and assumes the values \( \pm 1 \). We now write up this Hamiltonian in the ribbon geometry and perform and Fourier transform just like we did for the static Hamiltonian in Appendix A.3. Since the Hamiltonian in Eq. (A.6.1) is similar to the first term in the Haldane model accept for the additional phase we can read off what the dynamical Hamiltonian should read in the strip coordinates:

\[ H(t) = J_1 \sum_{j=1}^{N} \sum_{n=-\infty}^{\infty} \left( e^{iA_2j-1,n,2j,n}(t)c_{2j-1,n}^\dagger c_{2j,n} + \text{h.c.} \right) + J_1 \sum_{j=1}^{N} \sum_{n=-\infty}^{\infty} \left( e^{iA_2j-1,n,2j-1,n}(t)c_{2j-1,n}^\dagger c_{2j,n-1} + \text{h.c.} \right) + J_1 \sum_{j=1}^{N} \sum_{n=-\infty}^{\infty} \left( e^{iA_2j,n,2j+1,n}(t)c_{2j,n}^\dagger c_{2j+1,n} + \text{h.c.} \right). \]  

(A.6.2)

Fourier transforming we obtain:

\[ H(t) = \frac{J_1}{N} \sum_{k_y,k_y'} \sum_{j=1}^{N} \sum_{n=-\infty}^{\infty} \left( e^{i\frac{\pi}{2} A(t)} \delta_k c_{2j-1,k_y}^\dagger c_{2j,k_y'} \mathbf{e}^{i(k_y - k_y') \mathbf{r}_{2j-1,n} - i(k_y' - k_y) \mathbf{r}_{2j,n} + \text{h.c.}} \right) \]  

\[ + \frac{J_1}{N} \sum_{k_y,k_y'} \sum_{j=1}^{N} \sum_{n=-\infty}^{\infty} \left( e^{i\frac{\pi}{2} A(t)} \delta_k c_{2j-1,k_y}^\dagger c_{2j,k_y'} \mathbf{e}^{i(k_y - k_y') \mathbf{r}_{2j-1,n} - i(k_y' - k_y) \mathbf{r}_{2j,n-1} + \text{h.c.}} \right) \]  

\[ + \frac{J_1}{N} \sum_{k_y,k_y'} \sum_{j=1}^{N} \sum_{n=-\infty}^{\infty} \left( e^{i\frac{\pi}{2} A(t)} (-\delta_k) c_{2j,k_y}^\dagger c_{2j+1,k_y'} \mathbf{e}^{i(k_y - k_y') \mathbf{r}_{2j,n} - i(k_y' - k_y) \mathbf{r}_{2j+1,n} + \text{h.c.}} \right). \]  

(A.6.3)

We now use the relations:

\[ \mathbf{r}_{2j-1,n} - \mathbf{r}_{2j,n} = \delta_1 , \quad \mathbf{r}_{2j-1,n} - \mathbf{r}_{2j,n-1} = \delta_2 , \quad \mathbf{r}_{2j,n} - \mathbf{r}_{2j+1,n} = -\delta_3 \]  

(A.6.4)
The Hamiltonian in Eq. (A.6.3) can then be written as

\[
H(t) = J_{1} \sum_{k_{y}} \sum_{j=1}^{\frac{L}{2}} (e^{-i(k_{y} - \frac{\pi}{2} A(t)) \delta A_{j}} c_{j-1,k_{y}}^{\dagger} c_{j,k_{y}} + \text{h.c.}) \\
+ J_{1} \sum_{k_{y}} \sum_{j=1}^{\frac{L}{2}} (e^{-i(k_{y} - \frac{\pi}{2} A(t)) \delta A_{j}} c_{j-1,k_{y}}^{\dagger} c_{j,k_{y}} + \text{h.c.}) \\
+ J_{1} \sum_{k_{y}} \sum_{j=1}^{\frac{L}{2}-1} (e^{i A(t) (-\delta A_{j})} c_{j,k_{y}}^{\dagger} c_{j+1,k_{y}} + \text{h.c.}).
\]

(A.6.5)

The last term does not pick up any momentum dependent phase since \(\delta A\) is perpendicular to \(k_{y}\). Note that the result in Eq. (A.6.5) is exactly what we would have expected from minimal coupling, namely that we should make the substitution \(k_{y} \rightarrow k_{y} - \frac{\pi}{2} A(t)\). In order to study the driven system we wish to find the Fourier components of the time dependent Hamiltonian in Eq. (A.6.5) we can then subsequently compute various Greens functions and local observables using the extended space formalism. The integrals cannot be carried out directly as they are written in Eq. (A.6.5). First we make use of the so called Jacobi-Anger expansion [50]:

\[
e^{iz \cos(\phi)} = \sum_{m=-\infty}^{\infty} i^{m} J_{m}(z) e^{im \phi}
\]

where \(z\) is a complex number and \(J_{m}(z)\) denotes the bessel functions of the first kind. First we write the time dependent phases in Eq. (A.6.5):

\[
e^{i A(t) \delta_{1}} = e^{i \frac{\pi}{2} \delta_{1} (\cos(\Omega t) + \frac{\pi}{2} \rho \sin(\Omega t))} = e^{i \lambda (\cos(\pi/3) \cos(\Omega t) + \rho \sin(\pi/3) \sin(\Omega t))} = e^{i \lambda (\cos(\pi/3 - \rho \Omega t))}
\]

where we introduced the dimensionless constant \(\lambda = \frac{\pi \omega A}{\hbar}\). The 2 remaining phases are given by:

\[
e^{i A(t) \delta_{2}} = e^{i \lambda (\cos(\pi/3 - \rho \Omega t))}, \quad e^{-i A(t) \delta_{3}} = e^{i (\lambda \cos(\Omega t))}
\]

(A.6.8)

Applying the Jacobi-Anger expansion we get the Fourier components of the Hamiltonian in Eq. (A.6.5):

\[
H_{u} = \frac{1}{T} \int_{0}^{T} dt H(t) e^{-i n \rho \Omega t} = J_{1} \sum_{k_{y}} \sum_{j=1}^{\frac{L}{2}} \left( e^{-i \frac{\pi}{2} k_{y} a^{\dagger}_{j-1,k_{y}} c_{j,k_{y}}} \left[ \sum_{m=-\infty}^{\infty} i^{m} e^{i m \frac{\pi}{2} J_{m}(-\lambda)} \frac{1}{T} \int_{0}^{T} dt e^{i(n-m) \rho \Omega t} \right] \\
+ e^{-i \frac{\pi}{2} k_{y} a^{\dagger}_{j-1,k_{y}} c_{j,k_{y}}} \left[ \sum_{m=-\infty}^{\infty} i^{m} e^{i m \frac{\pi}{2} J_{m}(\lambda)} \frac{1}{T} \int_{0}^{T} dt e^{i(n-m) \rho \Omega t} \right] \right) \\
+ J_{1} \sum_{k_{y}} \sum_{j=1}^{\frac{L}{2}} \left( e^{-i \frac{\pi}{2} k_{y} a^{\dagger}_{j-1,k_{y}} c_{j,k_{y}}} \left[ \sum_{m=-\infty}^{\infty} i^{m} e^{i m \frac{\pi}{2} J_{m}(-\lambda)} \frac{1}{T} \int_{0}^{T} dt e^{i(n-m) \rho \Omega t} \right] \\
+ e^{-i \frac{\pi}{2} k_{y} a^{\dagger}_{j-1,k_{y}} c_{j,k_{y}}} \left[ \sum_{m=-\infty}^{\infty} i^{m} J_{m}(\lambda) \frac{1}{T} \int_{0}^{T} dt e^{i(n+m) \rho \Omega t} \right] \right) \\
+ C_{2j,k_{y}}^{\dagger} c_{j+1,k_{y}} \left[ \sum_{m=-\infty}^{\infty} i^{m} J_{m}(\lambda) \frac{1}{T} \int_{0}^{T} dt e^{i(n+m) \rho \Omega t} \right] \\
+ C_{2j,k_{y}}^{\dagger} c_{j+1,k_{y}} \left[ \sum_{m=-\infty}^{\infty} i^{m} J_{m}(-\lambda) \frac{1}{T} \int_{0}^{T} dt e^{i(n+m) \rho \Omega t} \right].
\]

(A.6.9)
Which reduces to:

\[
H_n = J_1 \sum_{k_y} \sum_{j=1}^{\frac{L}{2}} \left( e^{-i \frac{2\pi}{L} k_y a c_{2j-1,k_y}^\dagger c_{2j,k_y}} (e^{i \frac{2\pi}{L}})^{\nu} J_n (\lambda) + e^{i \frac{2\pi}{L} k_y a c_{2j,k_y}^\dagger c_{2j-1,k_y}} (e^{i \frac{2\pi}{L}})^{\nu} J_n (\lambda) \right)
\]

\[
+ J_1 \sum_{k_y} \sum_{j=1}^{\frac{L}{2}} \left( e^{i \frac{2\pi}{L} k_y a c_{2j,k_y}^\dagger c_{2j+1,k_y}} (e^{i \frac{2\pi}{L}})^{\nu} J_n (\lambda) + e^{-i \frac{2\pi}{L} k_y a c_{2j,k_y}^\dagger c_{2j+1,k_y}} (e^{i \frac{2\pi}{L}})^{\nu} J_n (\lambda) \right)
\]

\[
= J_1 \sum_{k_y} \sum_{j=1}^{\frac{L}{2}} \left( \left( e^{-i \frac{2\pi}{L} k_y a - n \rho \frac{2\pi}{3}} J_n (\lambda) + e^{i \frac{2\pi}{L} k_y a + n \rho \frac{2\pi}{3}} J_n (\lambda) \right) c_{2j-1,k_y}^\dagger c_{2j,k_y}
\]

\[
+ \left( e^{i \frac{2\pi}{L} k_y a + n \rho \frac{2\pi}{3}} J_n (\lambda) + e^{-i \frac{2\pi}{L} k_y a - n \rho \frac{2\pi}{3}} J_n (\lambda) \right) c_{2j-1,k_y}^\dagger c_{2j,k_y}
\]

\[
+ J_1 \sum_{k_y} \sum_{j=1}^{\frac{L}{2} - 1} \left( c_{2j,k_y}^\dagger c_{2j+1,k_y} i^{-n} J_n (\lambda) + c_{2j,k_y}^\dagger c_{2j+1,k_y} i^{-n} J_n (\lambda) \right)
\]

(A.6.10)

Rearranging the phases we get:

\[
H_n = \sum_{k_y} \sum_{j=1}^{\frac{L}{2}} \left( 2 \cos \left( \frac{\sqrt{3}}{2} k_y a - n \rho \frac{2\pi}{3} \right) e^{i n \rho \frac{2\pi}{3}} J_n (\lambda) c_{2j-1,k_y}^\dagger c_{2j,k_y}
\]

\[
+ 2 \cos \left( \frac{\sqrt{3}}{2} k_y a + n \rho \frac{2\pi}{3} \right) e^{i n \rho \frac{2\pi}{3}} J_n (\lambda) c_{2j-1,k_y}^\dagger c_{2j,k_y}
\]

\[
+ J_1 \sum_{k_y} \sum_{j=1}^{\frac{L}{2} - 1} \left( c_{2j,k_y}^\dagger c_{2j+1,k_y} i^{-n} J_n (\lambda) + c_{2j,k_y}^\dagger c_{2j+1,k_y} i^{-n} J_n (\lambda) \right)
\]

(A.6.11)

where we defined the effective hopping parameter \( J_{\rho(n)} (\lambda) = J_1 J_{\rho(n)} (\lambda) \). So far everything is exact. Of course when we do actual numerical calculations the number of harmonics \( H_n \) we need to keep depends on the driving amplitude and therefore the weekly driven limit is easier to access since it requires fewer copies.
Appendix B

Derivations for Chapter 4

B.1 Heisenberg equation of motion for the number operator

To evaluate the expression for the current in Eq. (4.1.6) we use the Heisenberg equation of motion:

\[-e\langle \dot{N}_L(t) \rangle = -\frac{ie}{\hbar} \langle U^\dagger(t,0)[H(t),N_L(0)]U(t,0) \rangle.\]

(B.1.1)

To proceed we evaluate the commutator:

\[ [H(t),N_L(0)] = \sum_{\alpha \in L} \sum_{\alpha' \in L,R} \epsilon_{\alpha'\alpha}[c^\dagger_{\alpha'}c_{\alpha'},c^\dagger_{\alpha}c_{\alpha}] + \sum_{\alpha \in L} \sum_{mn} h_{mn}(t)[d^\dagger_{m}d_{n},c^\dagger_{\alpha}c_{\alpha}] \]

(B.1.2)

\[ + \sum_{\alpha \in L} \sum_{\alpha' \in L,R} n_{\alpha'}(-V_{\alpha',n})c^\dagger_{\alpha'}d_{n}\delta_{\alpha\alpha'} + \sum_{\alpha \in L} \sum_{\alpha' \in L,R} V^*_{\alpha',n}d^\dagger_{n}c_{\alpha}\delta_{\alpha\alpha'} \]

(B.1.3)

\[ [H(t),N_L(0)] = \sum_{\alpha \in L} ((-V_{\alpha,n})c^\dagger_{\alpha}d_{n} + V^*_{\alpha,n}d^\dagger_{n}c_{\alpha}). \]

(B.1.4)

We now use Eq. (B.1.1) and Eq. (B.1.5) to get the current

\[ J_L = \frac{ie}{\hbar} \sum_{\alpha \in L} V_{\alpha,n}[c^\dagger_{\alpha}(t)d_{n}(t)] - V^*_{\alpha,n}[d^\dagger_{n}(t)c_{\alpha}(t)]. \]

(B.1.6)

B.2 Analytic continuation via Langreth rules

Here we illustrate how to use the Langreth method to perform analytic continuation. Many different identities can be derived this way and I won’t state them all here. However the method applied can be extended to any type of contour-defined quantity. Consider the contour ordered quantity \( C^c(\tau, \tau') \). We choose to apply the analytic continuation scheme to the lesser component which is given by:

\[ C^c(t_1, t_2) = \int_C d\tau A(t_1, \tau)B(\tau, t_2). \]

(B.2.1)

We now deform the contour Keldysh contour \( C \) such that it has two parts, see Fig. B.1.
An additional step has been added to the contour such that it runs back to $\tau = -\infty$ and then up to $\tau = \infty$. Now the equation for $C^<(t_1, t_2)$ can be written as

$$C^<(t_1, t_2) = \int_{C_1} d\tau A(t_1, \tau) B^<(\tau, t_2) + \int_{C_2} d\tau A^<(t_1, \tau) B(\tau, t_2). \quad (B.2.2)$$

Each of these can then be expressed in terms of the real time variable $t$ by splitting the contours in two parts. For the first term this procedure works in the following way

$$\int_{C_1} d\tau A(t_1, \tau) B^<(\tau, t_2) = \int_{-\infty}^{t_1} dtA(t_1, t)B^<(t, t_2) + \int_{t_1}^{\infty} dtA(t_1, t)B^<(t, t_2) \quad (B.2.3)$$

Now for the first integral $t_1 > t$ and for the second integral $t_1 < t$, therefore we add a $>$ to $A(t_1, t)$ in the first term and a $<$ to $A(t_1, t)$ in the second term:

$$\int_{C_1} d\tau A(t_1, \tau) B^<(\tau, t_2) = \int_{-\infty}^{\infty} dtA^>(t_1, t)B^<(t, t_2) + \int_{-\infty}^{t_1} dtA^<(t_1, t)B^<(t, t_2)$$

$$= \int_{-\infty}^{t_1} dtA^>(t_1, t)B^<(t, t_2) - \int_{-\infty}^{t_1} dtA^<(t_1, t)B^<(t, t_2)$$

$$= \int_{-\infty}^{\infty} dt\theta(t_1 - t)A^>(t_1, t)B^<(t, t_2) - \int_{-\infty}^{\infty} dt\theta(t_1 - t)A^<(t_1, t)B^<(t, t_2)$$

$$\quad = \int_{-\infty}^{\infty} dtA^r(t_1, t)B^<(t, t_2), \quad (B.2.4)$$

where we used that $A^r(t_1, t) = \theta(t_1 - t) (A^>(t_1, t) - A^<(t_1, t))$. Performing a similar calculation for the contour $C_2$ yields

$$\int_{C_2} d\tau A^<(t_1, \tau) B(\tau, t_2) = \int_{-\infty}^{\infty} dtA^<(t_1, t)B^a(t, t_2). \quad (B.2.5)$$

The final result is then

$$C^<(t_1, t_2) = \int_{-\infty}^{\infty} dt (A^r(t_1, t)B^<(t, t_2) + A^<(t_1, t)B^a(t, t_2)). \quad (B.2.6)$$

This may be used to find for instance the non-equilibrium lesser Green’s function. A table of Langreth rules is listed in Fig. (B.2).
B.3 Expressions for $G^r$ and $\Sigma^r$

We wish to derive an expression for the retarded Green’s function $G^r$. To do so we start by finding the retarded component of the contour-ordered Green’s function $G^c$. To do so we write up the contour-ordered Green’s function in the Larkin Ovchinnikov basis introduced in the main text. The Dyson equation for $G^r$ then becomes:

\[
G^r = (G^c)_{11} = (G^c)_{11} + (G^c_0 \otimes \Sigma^c \otimes G^c)_{11} = G^c + \left( \begin{bmatrix} G^c_0 & G^c_k \end{bmatrix} \otimes \begin{bmatrix} \Sigma^c_r & \Sigma^c_k \end{bmatrix} \otimes \begin{bmatrix} G^c_r & G^c_a \end{bmatrix} \right)_{11} \tag{B.3.1}
\]

\[
= G^c_0 + \left( \begin{bmatrix} G^c_0 \otimes \Sigma^c_r \otimes G^c & G^c_0 \otimes \Sigma^c_a \otimes G^c \end{bmatrix} \right)_{11} = G^c_0 + G^c_0 \otimes \Sigma^c \otimes G^c.
\tag{B.3.2}
\]

We can also write Eq. (B.3.2) as integro-differential equation:

\[
G^r_0^{-1} \circ G^r = \mathbb{1} + \Sigma^r \circ G^r
\tag{B.3.3}
\]

This form of the Dyson equation will be useful at some later stage when we want to solve Eq. (B.3.3) to obtain $G^r(t,t')$. For now we will try to explicitly obtain the expression for the self-energy $\Sigma^r$ in Eq. (B.3.3). To do so we find an equation of motion for $G^r(t,t')$. We can then compare our result with the result in Eq. (B.3.3). By comparison we will be able to read off what the self energy is. We start by finding an equation of motion for $G^r(t,t')$:

\[
i \frac{d}{dt} G^r(t,t') = \delta(t-t') + H(t)G^r(t,t') + V^\dagger c(t).
\tag{B.3.4}
\]

The equation of motion for $G^r(t,t')$ then becomes:

\[
i \frac{d}{dt} G^r(t,t') = \delta(t-t') + H(t)G^r(t,t') + V^\dagger G^r(t,t'),
\tag{B.3.5}
\]

where we have defined:

\[
G^r(t,t') = -i\theta(t-t')\{c(t),d^\dagger(t')\}.
\tag{B.3.6}
\]

To decouple the differential equation in Eq. (B.3.5) we need to find an equation for $\Sigma^r(t,t')$. To do so we start by finding $i \frac{d}{dt} G^r(t,t')$:

\[
i \frac{d}{dt} G^r(t,t') = -i\theta(t-t')\{i \frac{d}{dt} c(t),d^\dagger(t')\}.
\tag{B.3.7}
\]

To evaluate $i \frac{d}{dt} c(t)$ we apply the Heisenberg equation of motion:

\[
i \frac{d}{dt} c(t) = H_c c(t) + V d(t).
\tag{B.3.8}
\]
We now insert this expression into Eq. (B.3.7) to obtain:

\[ i \frac{d}{dt} \mathcal{G}'(t, t') = H_c \mathcal{G}'(t, t') + V \mathcal{G}'(t, t'), \tag{B.3.9} \]

We now rearrange the terms in Eq. (B.3.9) to get:

\[ (g_0^c(t))^{-1} \mathcal{G}'(t, t') = V \mathcal{G}'(t, t'), \tag{B.3.10} \]

where we defined:

\[ (g_0^c(t))^{-1} = i \frac{d}{dt} - H_c \tag{B.3.11} \]

we now apply \( g^c \) from the left on both sides of Eq. (B.3.10) to obtain:

\[ g^c = g_0^c \circ V \mathcal{G}'. \tag{B.3.12} \]

We now insert the expression in Eq. (B.3.12) into Eq. (B.3.5) to obtain:

\[ i \frac{d}{dt} \mathcal{G}'(t, t') = \delta(t - t') + H_S(t) \mathcal{G}'(t, t') + \int_{-\infty}^{\infty} dt_1 V^{\dagger} g_0^c(t - t_1) V \mathcal{G}'(t_1, t'). \tag{B.3.13} \]

We now rearrange the terms in Eq. (B.3.13) to get:

\[ \left( i \frac{d}{dt} - H_S(t) \right) \mathcal{G}'(t, t') = \delta(t - t') + \int_{-\infty}^{\infty} dt_1 V^{\dagger} g_0^c(t - t_1) V \mathcal{G}'(t_1, t'). \tag{B.3.14} \]

We now have an exact expression for the retarded Green’s function. By comparison with Eq. (B.3.2) we see that the retarded self energy in this case is given by

\[ \Sigma'(t, t') = V^{\dagger} g_0^c(t - t') V \tag{B.3.15} \]

Since the leads are not driven the bare Green’s function \( g_0^c(t - t') \) only depends on the time difference and therefore so does the self energy. We may therefore write \( \Sigma'(t, t') = \Sigma'(t - t') \). By changing time coordinate \( \tau = t - t_1 \) we get

\[ \left( i \frac{d}{dt} - H_S(t) \right) \mathcal{G}'(t, t') = \delta(t - t') - \int_{-\infty}^{\infty} d\tau \Sigma'(\tau) \mathcal{G}'(t - \tau, t') = \delta(t - t'). \tag{B.3.16} \]

Taking the Fourier transform of \( \mathcal{G}'(t, t') \) on the left is not straightforward since the derivative \( i \frac{d}{dt} \) is in a variable different from \( t' \) which is the variable in which we take the Fourier transform. To see how this works we use the definition in Eq. (4.2.18) and apply it to the term with a derivative in Eq. (B.7.12) to get:

\[ \int_{-\infty}^{\infty} dt' \left( i \frac{d}{dt} \mathcal{G}'(t, t') \right) e^{-i\xi(t' - t)} = i \frac{d}{dt} \int_{-\infty}^{\infty} dt' \mathcal{G}'(t, t') e^{-i\xi(t' - t)} + \xi \int_{-\infty}^{\infty} dt' \mathcal{G}'(t, t') e^{-i\xi(t' - t)} \]

\[ = i \frac{d}{dt} \mathcal{G}'(t, \xi) + \xi \mathcal{G}'(t, \xi), \tag{B.3.17} \]

where I used partial integration. To get the Fourier transform of the last term on the left hand side of Eq. (B.3.16) we first express \( \mathcal{G}'(t - \tau, t') \) in terms of the inverse Fourier transform

\[ \mathcal{F} \left( \int_{-\infty}^{\infty} d\tau \Sigma'(\tau) \mathcal{G}'(t - \tau, t') \right) \]

\[ = \int_{-\infty}^{\infty} dt' e^{-i\xi(t' - t)} \int_{-\infty}^{\infty} d\tau \Sigma'(\tau) \mathcal{G}'(t - \tau, t') \]

\[ = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\xi' \int_{-\infty}^{\infty} dt' e^{-i\xi(t' - t)} \int_{-\infty}^{\infty} d\tau \Sigma'(\tau) \mathcal{G}'(t - \tau, \xi') e^{i\xi'(t' - t + \tau)}. \tag{B.3.18} \]

By using these results we can write the Fourier transform of the equation of motion (B.3.16) as

\[ \left( i \frac{d}{dt} + \xi - H_S(t) \right) \mathcal{G}'(t, \xi) - \int_{-\infty}^{\infty} d\tau \Sigma'(\tau) \mathcal{G}'(t - \tau, \xi) = 0. \tag{B.3.19} \]
B.4 Retarded Floquet Green’s function in the Floquet basis

We start by rewriting the equation of motion from Eq. (4.2.25) in the main text

$$\left( \mathcal{E} + i \frac{d}{dt} - \tilde{H}_S(t) \right) G^r(t, \mathcal{E}) = I. \quad (B.4.1)$$

We wish to find a solution for $G^r(t, \mathcal{E})$ in terms of Floquet states. We know from Chapter 1 that Floquet states are eigenvalues of the Floquet operators. However the Hamiltonian in the equation of motion has a non-Hermitian part. It is still possible to find eigenstates in that case we simply have to introduce a bi-orthogonal basis. In that case the modified eigenvalue equation becomes

$$\left( \mathcal{E} + i \frac{d}{dt} - (H_S(t) \pm i \Gamma) \right) |\phi_\alpha^\pm(t)\rangle = (-\epsilon_\alpha \mp i \gamma_\alpha) |\phi_\alpha^\pm(t)\rangle, \quad (B.4.2)$$

where $|\phi_\alpha^\pm(t)\rangle$ is the right eigenstate with eigenvalue $\epsilon_\alpha \pm i \gamma_\alpha$. For each right eigenket there is a left eigenbra which satisfy

$$\langle \phi_\alpha^\pm(t)| \left( \mathcal{E} + i \frac{d}{dt} - (H_S(t) \mp i \Gamma) \right) = \langle \phi_\alpha^\pm(t)| (-\epsilon_\alpha \mp i \gamma_\alpha). \quad (B.4.3)$$

Together the left/right eigenket/eigenbra forms the bi-orthogonal basis

$$\sum_\alpha |\phi_\alpha^-(t)\rangle \langle \phi_\alpha^+(t)| = \mathbb{I}. \quad (B.4.4)$$

An ansatz for $G^r(t, \mathcal{E})$ is then

$$G^r(t, \mathcal{E}) = \sum_\alpha |\phi_\alpha^-(t)\rangle \langle \phi_\alpha^+(t)| / (\mathcal{E} - \epsilon_\alpha + i \gamma_\alpha). \quad (B.4.5)$$

We can now find the retarded Floquet Green’s functions by applying Eq. (4.2.21) from the main text and by expanding the Floquet states in terms of their harmonics:

$$G^{r(n)}(\mathcal{E}) = \frac{1}{T} \int_0^T dt G^r(t, \mathcal{E}) e^{i n \Omega t} \quad (B.4.6)$$

$$= \frac{1}{T} \int_0^T dt \sum_{m,k=\infty}^\infty \sum_\alpha |\phi_\alpha^{-m}(k)\rangle \langle \phi_\alpha^{+m}| \frac{1}{\mathcal{E} - \epsilon_\alpha + i \gamma_\alpha} e^{i (n+m-k) \Omega t}$$

$$= \sum_{m=-\infty}^\infty \sum_\alpha |\phi_\alpha^{-m}(m)\rangle \langle \phi_\alpha^{+m}| / (\mathcal{E} - m \Omega - \epsilon_\alpha + i \gamma_\alpha). \quad (B.4.7)$$

In terms of real energies $E_\alpha = \epsilon_\alpha + m \Omega$ the retarded Floquet Green’s function is

$$G^{r(n)}(\mathcal{E}) = \sum_{m=-\infty}^\infty \sum_\alpha |\phi_\alpha^{-m}(m)\rangle \langle \phi_\alpha^{+m}| / (\mathcal{E} - m \Omega - E_\alpha + i \gamma_\alpha). \quad (B.4.8)$$

B.5 Expression for the lesser Green’s function $G^<$

In order to get the lesser Green’s function $G^<(t, t')$ we first need to find the contour ordered Green’s function $G^<(\tau, \tau')$. When this is determined we can find the lesser Green’s function using the Langreth method described in the main text. In order to find the contour-ordered Green’s function we start by finding the time-ordered Green’s function:

$$G^T_{n,\alpha}(t - t_1) = -i \langle T \{ \hat{c}_{\alpha}^\dagger(t_1), d_\alpha(t) \} \rangle \quad (B.5.1)$$

The equation of motion for the time-ordered Green’s function becomes:

$$-i \frac{d}{dt_1} G^T_{n,\alpha}(t - t_1) = -i \langle T \{ -i \frac{d}{dt_1} \hat{c}_{\alpha}^\dagger(t_1), d_\alpha(t) \} \rangle. \quad (B.5.2)$$

In principle there is an additional term from taking the derivatives of the Heaviside step functions in the time ordering operator. However this gives an equal times commutator between the operators $d_\alpha$ and $\hat{c}_{\alpha}^\dagger$.
Using the result in Eq. (B.5.6) we can now write Eq. (B.5.3) as:

$$-i \frac{d}{dt_1} c^\dagger_\alpha (t_1) = U(t_1,0) [H(t_1), c^\dagger_\alpha] U^\dagger(t_1,0)$$

(B.5.3)

$$[H(t_1), c^\dagger_\alpha] = \sum_{m,j} h_{mj}(t_1) [d^*_m dt, c^\dagger_\alpha] + \sum_{\alpha'} \epsilon_\alpha [c^\dagger_{\alpha'}, c^\dagger_\alpha]$$

(B.5.4)

$$+ \sum_{\alpha',m} \left( V_{\alpha',m} c^\dagger_{\alpha',m} d_m + V_{\alpha',m} d^*_m c^\dagger_{\alpha',m} \right)$$

(B.5.5)

$$= \epsilon_\alpha c_\alpha + \sum_m V^*_{\alpha,m} d_m$$

(B.5.6)

Using the result in Eq. (B.5.6) we can now write Eq. (B.5.3) as:

$$-i \frac{d}{dt_1} c^\dagger_\alpha (t_1) = \epsilon_\alpha c_\alpha (t_1) + \sum_m V^*_{\alpha,m} d_m (t_1)$$

(B.5.7)

The equation of motion in Eq. (B.5.2) then reads

$$- \frac{d}{dt_1} G^\alpha_{n,m}(t_t-t_1) = \epsilon_\alpha (-i) \langle T \{ -i \frac{d}{dt_1} c^\dagger_{\alpha}(t_1), d_n(t) \} \rangle + \sum_m V^*_{\alpha,m} (-i) \langle T \{ d_m(t_1), d_n(t) \} \rangle$$

(B.5.8)

$$\left( -i \frac{d}{dt_1} - \epsilon_\alpha \right) G^\alpha_{n,m}(t_t-t_1) = \sum_m G^T_{nm}(t_t-t_1) V^*_{\alpha,m}$$

(B.5.9)

We now multiply both sides of Eq. (B.5.9) from the right with $g^T_{0\alpha}(t_1-t')$ and integrate on both sides of the equation with respect to the variable $t_1$:

$$\int_{-\infty}^{\infty} dt_1 (-i \frac{d}{dt_1} - \epsilon_\alpha) G^T_{n,m}(t_t-t_1) g^T_{0\alpha}(t_1-t') = \int_{-\infty}^{\infty} dt_1 \sum_m G^T_{nm}(t_t-t_1) V^*_{\alpha,n}(t_1) g^T_{0\alpha}(t_1-t')$$

(B.5.10)

On the left hand side of Eq. (B.5.10) the derivative acts on $G^\alpha_{n,m}(t_t-t_1)$. By performing partial integration we can let it act on $g^T_{0\alpha}(t_1-t')$ instead. Eq. (B.5.10) then becomes:

$$\int_{-\infty}^{\infty} dt_1 G^T_{n,m}(t_t-t_1)(i \frac{d}{dt_1} - \epsilon_\alpha) g^T_{0\alpha}(t_1-t') = \int_{-\infty}^{\infty} dt_1 \sum_m G^T_{nm}(t_t-t_1) V^*_{\alpha,m} g^T_{0\alpha}(t_1-t')$$

(B.5.11)

Due to the sign flip on the derivative in Eq. (B.5.11), we can now identify the factor multiplying $g^T_{0\alpha}(t_1-t')$ as the inverse of $g^T_{0\alpha}(t_1-t')$. That is it satisfies

$$g^T_{0\alpha}(t_1) = (i \frac{d}{dt_1} - \epsilon_\alpha), \quad g^T_{0\alpha}(t_1-t') = I.$$  

(B.5.12)

The expression in Eq. (B.5.11) then reads

$$G^T_{n,m}(t_t-t') = \int_{-\infty}^{\infty} dt_1 \sum_m G^T_{nm}(t_t-t_1) V^*_{\alpha,m} g^T_{0\alpha}(t_1-t').$$  

(B.5.13)

We now apply an argument given in the main text which is that the structure of the equilibrium time-ordered Green’s function and is similar to the non-equilibrium contour-ordered Green’s function with the only difference being that the non-equilibrium Green’s function has time arguments on the Keldysh contour. From inspection Eq. (B.5.13) we see that the contour-ordered Green’s function is then:

$$G^c_{n,m}(t_t,t') = \int_{-\infty}^{\infty} dt_1 \sum_m G^c_{nm}(t_t,t_1) V^c_{\alpha,m} g^c_{\alpha}(t_1-t').$$  

(B.5.14)

The lesser Green’s function is the upper right component of the contour-ordered Green’s function. In Appendix B.2 we used the Langreth method to perform analytic continuation. We now apply the result obtained there to the Green’s function in Eq. (B.5.14) to get:

$$G^c_{n,m}(t_t,t') = \int_{-\infty}^{\infty} dt_1 \sum_m V^c_{\alpha,m} \left( G^c_{nm}(t_t,t_1) g^c_{\alpha}(t_1,t') + G^c_{nm}(t_t,t_1) g^0_{\alpha}(t_1,t') \right).$$  

(B.5.15)
B.6 Expressions for $G^<$ and $\Sigma^<$

In this section we derive the full lesser Green’s function $G^<(t, t’)$ for the system. We start by writing up the Dyson equation for the contour Green’s function of the system

$$G^r = G^r_0 + G^r_0 \otimes \Sigma^c \otimes G^r.$$  \hspace{1cm} (B.6.1)

By applying the Langreth rule for $G^<$ we obtain an expression for the lesser Green’s function from the contour ordered Green’s function. The rule we need is listed in Fig. B.2 in Appendix B.2. Here we state the result:

$$G^< = G^<_0 + G^<_0 \circ \Sigma^c \circ G^a + G^r_0 \circ \Sigma^c \circ G^< + G^<_0 \circ \Sigma^c \circ G^a.$$  \hspace{1cm} (B.6.2)

$$G^< = G^<_0 \circ (\mathbb{I} + \Sigma^c \circ G^a) + G^r_0 \circ \Sigma^c \circ G^< + G^<_0 \circ \Sigma^c \circ G^a.$$  \hspace{1cm} (B.6.3)

$$(\mathbb{I} - G^r_0 \circ \Sigma^r) \circ G^< = G^<_0 \circ (\mathbb{I} + \Sigma^c \circ G^a) + G^r_0 \circ \Sigma^c \circ G^a.$$  \hspace{1cm} (B.6.4)

Using the Dyson equation for the retarded Green’s function we can obtain an expression for the retarded self-energy

$$G^r = G^r_0 + G^r_0 \circ \Sigma^c \circ G^r \Leftrightarrow \Sigma^r = G^r_0^{-1} - G^r.$$  \hspace{1cm} (B.6.5)

Eq. (B.6.4) can then be written as

$$G^r_0 \circ G^r_0^{-1} \circ G^< = G^<_0 \circ (\mathbb{I} + \Sigma^c \circ G^a) + G^r_0 \circ \Sigma^c \circ G^a.$$  \hspace{1cm} (B.6.6)

We then multiply with $G^r \circ G^r_0^{-1} \circ$ from the left on both sides of Eq. (B.6.6) to get:

$$G^< = G^r \circ G^r_0^{-1} \circ G^< \circ (\mathbb{I} + \Sigma^c \circ G^a) + G^r \circ \Sigma^c \circ G^a.$$  \hspace{1cm} (B.6.7)

The first term in Eq. (B.6.7) is actually zero. This follows from the fact that $G^r_0^{-1} \circ G^<_0$ is zero. This is straightforward to verify by writing out the definition. The full lesser Green’s function in Eq. B.6.7 then becomes (reinserting time arguments):

$$G^< = G^r \circ \Sigma^c \circ G^a,$$  \hspace{1cm} (B.6.8)

or equivalently with explicit time dependence.

$$G^<(t, t’) = \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 G^r(t, t_1) \Sigma^<(t_1, t_2) G^a(t_2, t’).$$  \hspace{1cm} (B.6.9)

The expression we have found for $G^<(t, t’)$ in Eq. (B.6.8) depends on the lesser self-energy. We now wish to get an explicit expression for the lesser self-energy in Eq. (B.6.8). To do so we apply the same procedure that we did for the retarded self energy. That is we start by finding an equation of motion for $G^<(t, t’) = i(d^<(t’)d(t))$. When we have a closed expression for $G^<(t, t’)$ we can then compare it with the expression in Eq. (B.6.8) and read off what the lesser self energy is. We start by finding an equation of motion for $G^<(t, t’)$:

$$i \frac{d}{dt} G^<(t, t’) = i(d^<(t’)i \frac{d}{dt} d(t))$$  \hspace{1cm} (B.6.10)

We have already found an expression for $i \frac{d}{dt} d(t)$ in Appendix (B.3) the result is:

$$i \frac{d}{dt} d(t) = H_S d(t) + V^c c(t).$$  \hspace{1cm} (B.6.11)

Plugging this into Eq. (B.6.10) we obtain:

$$i \frac{d}{dt} G^<(t, t’) = H_S G^<(t, t’) + V^c G^<(t, t’),$$  \hspace{1cm} (B.6.12)

where $G^<(t, t’) = i(d^<(t’)c(t))$. Note that this is different from the Green’s function $G^<$ defined in Appendix B.5 Rearranging terms in Eq. (B.6.12) we get:

$$G^<_0^{-1} G^<(t, t’) = V^c G^<(t, t’),$$  \hspace{1cm} (B.6.13)
where $G_0^{-1} = i \frac{d}{dt} - H_S(t)$. To get a closed equation for $G^<(t, t')$ we need an equation for $G^<(t, t')$. We start by finding the equation of motion for the time-ordered Green’s function $\mathcal{G}^T(t, t') = i(d^T(t')e(t))$:

$$i \frac{d}{dt} \mathcal{G}^T(t, t') = H, \mathcal{G}^T(t, t') + VG^T(t, t').$$  \hfill (B.6.14)

We now rearrange the terms in Eq. (B.6.14):

$$g_0^{-1}(t) \mathcal{G}^T(t, t') = VG^T(t, t') \Rightarrow \mathcal{G}^T = g_0^T \circ VG^T,$$  \hfill (B.6.15)

where $g_0^{-1}(t) = i \frac{d}{dt} - H_c$. As previously argued the non-equilibrium form is the same as in Eq. (B.6.15), the only difference being that the time integration runs on the Keldysh contour. From this argument we can then write the contour-ordered Green’s function as:

$$\mathcal{G}^c(\tau, \tau') = g_0^c \circ VG^c = \int_{-\infty}^{\infty} d\tau g_0^c(\tau, \tau_1) VG^c(\tau_1, \tau')$$  \hfill (B.6.16)

We now apply the Langreth rule for the lesser Green’s function (see table in Fig. B.2, Appendix B.2) to Eq. (B.6.16) to obtain the lesser component:

$$\mathcal{G}^< = g_0^c \circ VG^< + g_0^c \circ VG^a.$$  \hfill (B.6.17)

We now insert the expression in Eq. (B.6.17) into Eq. (B.6.13) to get:

$$G_0^{-1} \circ \mathcal{G}^< = V^\dagger g_0^c V \circ G^c + V^\dagger g_0^c V \circ G^a = \Sigma^r \circ \mathcal{G}^< + V^\dagger g_0^c V \circ G^a,$$  \hfill (B.6.18)

where we used the definition of the retarded self-energy obtained in Eq. (B.3.15). Isolating $\mathcal{G}^<$ in Eq. (B.6.18) we get

$$(G_0^{-1} - \Sigma^r) \circ \mathcal{G}^< = V^\dagger g_0^c V \circ G^a.$$  \hfill (B.6.19)

From the Dyson for the retarded self-energy obtained in Eq. (B.3.2) we see that $\Sigma^r = G_0^{-1} - G^r$. Inserting this into Eq. (B.6.19) we get:

$$G^r^{-1} \circ \mathcal{G}^< = V^\dagger g_0^c V \circ G^a.$$  \hfill (B.6.20)

Multiplying both sides of Eq. (B.6.20) by $G^r$ from the left yields

$$\mathcal{G}^< = G^r \circ V^\dagger g_0^c V \circ G^a.$$  \hfill (B.6.21)

If we compare Eq. (B.6.21) with Eq. (B.6.8) we see that the lesser self energy is given by:

$$\Sigma^< = V^\dagger g_0^c V.$$  \hfill (B.6.22)

We now apply an argument similar to that for $g_0^c(t - t')$. Since $g_0^c(t, t') = g_0^c(t - t')$, it follows from Eq. (B.6.22) that $\Sigma^<(t, t') = \Sigma^<(t - t')$.

**B.7 Expression for the time-averaged current $\langle J(t) \rangle$**

Our goal is to obtain an expression time averaged current using the JMW result from Eq. (4.3.11) in the main text. Since we are dealing with a periodically driven system we are only interested in the current averaged over one period:

$$\langle J_L(t) \rangle = -\frac{2e}{\hbar} \frac{1}{T} \int_0^T dt \int_{-\infty}^{\infty} d\xi \int_{-\infty}^{\infty} dt_1 \text{Im} \left[ e^{-i\xi(t_1-t)} \times \text{Tr} \left( \Gamma_L(\xi) \left( G^r(t, t_1)f_L(\xi) + G^<(t, t_1)\theta(t-t_1) \right) \right) \right],$$  \hfill (B.7.1)

where the brackets on the left hand side of the equality sign means that we are taking the time average over one period. By using the Floquet Green’s functions defined in the main text we can now derive an expression for the current in Eq. (B.7.1) in terms of the Fourier transform defined in Eq. (4.2.18):

$$\langle J_L(t) \rangle = -\frac{2e}{\hbar} \frac{1}{T} \int_0^T dt \int_{-\infty}^{\infty} d\xi \text{Im} \left[ \text{Tr} \left( \Gamma_L(\xi) \left( G^r(t, \xi)f_L(\xi) + G^<(t, \xi) \right) \right) \right],$$  \hfill (B.7.2)
where we have defined:

\[ G^< (t, \mathcal{E}) = \int_{-\infty}^{\infty} dt' G^< (t, t') e^{-i\mathcal{E}(t' - t)} \theta(t - t') = \int_{-\infty}^{\infty} ds G^< (t, t - s) e^{i\mathcal{E}s} \theta(s). \]  

(B.7.3)

We can simplify the expressions in the trace in Eq. (B.7.2) by using that \( \Gamma_L (\mathcal{E}) \) is Hermitian:

\[ \text{Im} \left[ \text{Tr} (\Gamma_L (\mathcal{E}) G^r (t, t') f_L (\mathcal{E})) \right] = \text{Tr} \left[ \text{Im} (\Gamma_L (\mathcal{E}) G^r (t, \mathcal{E})) f_L (\mathcal{E}). \right] \]  

(B.7.4)

Now define \( M = \Gamma_L (\mathcal{E}) G^r (t, \mathcal{E}). \) We can then write Eq. (B.7.4) as:

\[ \text{Tr} \left[ \text{Im} (\Gamma_L (\mathcal{E}) G^r (t, \mathcal{E})) \right] = \text{Tr} \left[ \text{Im} (M) \right] = \sum_j \frac{M_{jj} - (M^\dagger)_{jj}}{2i} = \frac{\sum_j (M_{jj} - (M^\dagger)_{jj})}{2i}. \]  

(B.7.5)

\[ = \sum_{jk} \left( \frac{G^r (t, \mathcal{E})_{jk} - (G^r (t, \mathcal{E})_{jk})^*}{2i} \right) \Gamma_{Ljk} (\mathcal{E}) = \text{Tr} \left[ \left( \frac{G^r (t, \mathcal{E}) - (G^r (t, \mathcal{E}))^\dagger}{2i} \right) \Gamma_L (\mathcal{E}) \right]. \]  

(B.7.6)

\[ = \sum_{jk} \left( \frac{G^r (t, \mathcal{E})_{jk} - (G^r (t, \mathcal{E})_{jk})^*}{2i} \right) \Gamma_{Ljk} (\mathcal{E}) = \text{Tr} \left[ \left( \frac{G^r (t, \mathcal{E}) - (G^r (t, \mathcal{E}))^\dagger}{2i} \right) \Gamma_L (\mathcal{E}) \right]. \]  

(B.7.7)

A similar analysis for the term in Eq. (B.7.2) containing \( G^< (t, \mathcal{E}) \) yields.

\[ \text{Tr} \left[ \text{Im} (\Gamma_L (\mathcal{E}) G^< (t, \mathcal{E})) \right] = \text{Tr} \left[ \left( \frac{G^< (t, \mathcal{E}) - (G^< (t, \mathcal{E}))^\dagger}{2i} \right) \Gamma_L (\mathcal{E}) \right]. \]  

(B.7.8)

The current in Eq. (B.7.2) then becomes

\[ \langle J_L (t) \rangle = \frac{2e}{\hbar} \frac{1}{T} \int_0^T dt \int_{-\infty}^{\infty} d\mathcal{E} \left( \text{Tr} \left[ \left( \frac{G^r (t, \mathcal{E}) - (G^r (t, \mathcal{E}))^\dagger}{2i} \right) \Gamma_L (\mathcal{E}) \right] f_L (\mathcal{E}) \right) \]  

\[ + \text{Tr} \left[ \left( \frac{G^< (t, \mathcal{E}) - (G^< (t, \mathcal{E}))^\dagger}{2i} \right) \Gamma_L (\mathcal{E}) \right]. \]  

(B.7.9)

To make things more manageable we first simplify the first trace in the formula above. We shall refer to this term as \( \langle J_L^1 (t) \rangle. \) The last term we refer to as \( \langle J_L^2 (t) \rangle. \) To simplify the first term in the current in Eq. (B.7.9) we start by writing up the Dyson equation for the retarded Green’s function \( G^r (t, t') \):

\[ G^r (t, t') = G^r_0 (t, t') + \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 G^r_0 (t, t_1) \Sigma^r (t_1, t_2) G^r (t_2, t'). \]  

(B.7.10)

We can rewrite this as a differential equation in \( G^r (t, t') \):

\[ G^r_0^{-1} (t) G^r (t, t') = \delta (t - t') + \int_{-\infty}^{\infty} dt_2 \Sigma^r (t, t_2) G^r (t_2, t'). \]  

(B.7.11)

We perform a change of variables to \( \tau = t - t_2. \) The equation then becomes:

\[ \left( i \frac{d}{dt} - H_S (t) \right) G^r (t, \tau) = \delta (t - \tau) + \int_{-\infty}^{\infty} d\tau \Sigma^r (\tau) G^r (t - \tau, t'). \]  

(B.7.12)

We wish to take Fourier transform defined in Eq. (4.2.18) of both sides of Eq. (B.7.12). Taking the Fourier transform of \( G^r (t, t') \) on the left is not straightforward since the derivative \( i \frac{d}{dt} \) is in a variable different from \( t' \) which is the variable in which we take the Fourier transform. To see how this works we use the definition in Eq. (4.2.18) and apply it to the term with a derivative in Eq. (B.7.12) to get:

\[ \int_{-\infty}^{\infty} dt' \left( i \frac{d}{dt} G^r (t, t') \right) e^{-i\mathcal{E}(t' - t)} = i \frac{d}{dt} \int_{-\infty}^{\infty} dt' G^r (t, t') e^{-i\mathcal{E}(t' - t)} + \mathcal{E} \int_{-\infty}^{\infty} dt' G^r (t, t') e^{-i\mathcal{E}(t' - t)} \]  

(B.7.13)

\[ = i \frac{d}{dt} G^r (t, \mathcal{E}) + \mathcal{E} G^r (t, \mathcal{E}), \]  

(B.7.14)
where I used partial integration. To get the Fourier transform of the last term on the right hand side of Eq. (B.7.12) we first express $G^r(t - \tau, t')$ in terms of the inverse Fourier transform

$$
\mathcal{F}\left(\int_{-\infty}^{\infty} dt' e^{-i\mathcal{E}'(t'-t)} \int_{-\infty}^{\infty} dt \Sigma^r(\tau) G^r(t - \tau, t')\right)
$$

$$
= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\mathcal{E}' \int_{-\infty}^{\infty} dt' e^{-i\mathcal{E}'(t'-t)} \int_{-\infty}^{\infty} dt \Sigma^r(\tau) G^r(t - \tau, \mathcal{E}') e^{i\mathcal{E}'(t'-t+\tau)}.
\tag{B.7.15}
$$

We now change variables to $s = t - t'$ and Eq. (B.7.15) then becomes:

$$
\frac{1}{2\pi} \int_{-\infty}^{\infty} d\mathcal{E}' \int_{-\infty}^{\infty} ds e^{i(s(\mathcal{E}' - \mathcal{E}))} \int_{-\infty}^{\infty} dt \Sigma^r(\tau) G^r(t - \tau, \mathcal{E}') e^{i\mathcal{E}'\tau}
\tag{B.7.16}
$$

$$
= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\mathcal{E}' 2\pi \delta(\mathcal{E} - \mathcal{E}') \int_{-\infty}^{\infty} dt \Sigma^r(\tau) G^r(t - \tau, \mathcal{E}') e^{i\mathcal{E}'\tau}
\tag{B.7.17}
$$

$$
= \int_{-\infty}^{\infty} dt \Sigma^r(\tau) G^r(t - \tau, \mathcal{E}) e^{i\mathcal{E}\tau}.
\tag{B.7.18}
$$

In conclusion we can write the Fourier transform of Eq. (B.7.12) as:

$$
\left(\frac{d}{dt} + \mathcal{E} - H_S(t)\right) G^r(t, \mathcal{E}) = \mathbb{I} + \int_{-\infty}^{\infty} dt \Sigma^r(\tau) G^r(t - \tau, \mathcal{E}) e^{i\mathcal{E}\tau}.
\tag{B.7.19}
$$

We obtain a similar equation for $(G^r(t, \mathcal{E}))^\dagger$ by taking the hermitian conjugate of Eq. (B.7.19):

$$
(G^r(t, \mathcal{E}))^\dagger \left(-i \frac{d}{dt} + \mathcal{E} - H_S(t)\right) G^r(t, \mathcal{E}) - (G^r(t, \mathcal{E}))^\dagger \int_{-\infty}^{\infty} dt \Sigma^r(\tau) G^r(t - \tau, \mathcal{E}) e^{i\mathcal{E}\tau}.
\tag{B.7.20}
$$

We now multiply Eq. (B.7.19) from the left with $(G^r(t, \mathcal{E}))^\dagger$ and rearrange the equation to obtain:

$$
(G^r(t, \mathcal{E}))^\dagger = (G^r(t, \mathcal{E}))^\dagger \left(-i \frac{d}{dt} + \mathcal{E} - H_S(t)\right) G^r(t, \mathcal{E}) - (G^r(t, \mathcal{E}))^\dagger \int_{-\infty}^{\infty} dt \Sigma^r(\tau) G^r(t - \tau, \mathcal{E}) e^{i\mathcal{E}\tau}.
\tag{B.7.21}
$$

We repeat this procedure for Eq. (B.7.20) which we multiply from the right with $G^r(t, \mathcal{E})$ and rearrange the terms to obtain:

$$
G^r(t, \mathcal{E}) = (G^r(t, \mathcal{E}))^\dagger \left(-i \frac{d}{dt} + \mathcal{E} - H_S(t)\right) G^r(t, \mathcal{E}) - \int_{-\infty}^{\infty} dt (G^r(t - \tau, \mathcal{E}))^\dagger \Sigma^r(\tau)^\dagger G^r(t, \mathcal{E}) e^{-i\mathcal{E}\tau}.
\tag{B.7.22}
$$

We can now evaluate the difference in Eq. (B.7.9) using Eq. (B.7.21) and Eq. (B.7.22):

$$
G^r(t, \mathcal{E}) - (G^r(t, \mathcal{E}))^\dagger = -i \frac{d}{dt} \left(\left(\frac{d}{dt} \mathcal{E} \right) \mathcal{E} \right) G^r(t, \mathcal{E}) - \int_{-\infty}^{\infty} dt (G^r(t - \tau, \mathcal{E}))^\dagger \Sigma^r(\tau)^\dagger G^r(t, \mathcal{E}) e^{-i\mathcal{E}\tau}
$$

$$
+ \int_{-\infty}^{\infty} dt (G^r(t, \mathcal{E}))^\dagger \Sigma^r(\tau) G^r(t - \tau, \mathcal{E}) e^{i\mathcal{E}\tau}.
\tag{B.7.23}
$$

The first term is just a total derivative so when we take the time average in Eq. (B.7.9) this term averages to zero. However for the non-average current this will no longer be true. Physically we may think of this term as charge running forth and back between the system and each lead. On average this process won’t contribute to the net current. However at a specific moment in time the current will change due to this process. Plugging Eq. (B.7.23) into the current in Eq. (B.7.9) the first term becomes:

$$
\langle J^L(t) \rangle = -\frac{2e}{h} \frac{1}{T} \int_{0}^{T} dt \int_{-\infty}^{\infty} d\mathcal{E} \int_{-\infty}^{\infty} dt \text{Tr} \left[ \text{Im} \left( (G^r(t, \mathcal{E}))^\dagger \Sigma^r(\tau) G^r(t - \tau, \mathcal{E}) e^{i\mathcal{E}\tau} \right) \Gamma_L(\mathcal{E}) \right] f_L(\mathcal{E}).
\tag{B.7.24}
$$
We can now express the Green’s functions using the Fourier decomposition in Eq. (4.2.20). The current in Eq. (B.7.24) then becomes:

$$\langle J^r_L(t) \rangle = \frac{-2e}{\hbar} \sum_{n,m=-\infty}^{\infty} \frac{1}{T} \int_0^T dt e^{i(n-m)t} \int_{-\infty}^{\infty} d\epsilon \left[ \text{Im} \left( (G^{(n)}(\epsilon))^\dagger \left( \int_{-\infty}^{\infty} d\tau \Sigma^r(\tau) e^{i(\epsilon + m\Omega)\tau} \right) G^{(m)}(\epsilon) \right) \Gamma_L(\epsilon) \right] f_L(\epsilon). \quad (B.7.25)$$

The term in parenthesis is just the Fourier transform of the retard self-energy. The current in Eq. (B.7.25) then becomes:

$$\langle J^r_L(t) \rangle = \frac{-2e}{\hbar} \sum_{n,m=-\infty}^{\infty} \delta_{n,m} \int_{-\infty}^{\infty} d\epsilon \text{Tr} \left[ \text{Im} \left( (G^{(n)}(\epsilon))^\dagger \left( \sum_r \Sigma^r(\epsilon + n\Omega) G^{(m)}(\epsilon) \right) \Gamma_L(\epsilon) \right) f_L(\epsilon) \right] \quad (B.7.26)$$

$$= \frac{-2e}{\hbar} \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} d\epsilon \text{Tr} \left[ (G^{(n)}(\epsilon))^\dagger \left( \sum_r \Sigma^r(\epsilon + n\Omega) - \frac{\Sigma^r(\epsilon + n\Omega)}{2i} G^{(n)}(\epsilon) \Gamma_L(\epsilon) \right) f_L(\epsilon) \right]. \quad (B.7.27)$$

In Appendix (B.3), the self energy $\Sigma^r(t,t')$ is found. The result is:

$$\Sigma^r(t,t') = V^\dagger g^r_0(t-t') V. \quad (B.7.28)$$

Since the leads are not driven the bare Green’s function $g^r_0(t-t')$ only depends on the time difference and therefore so does the self energy. We may therefore write $\Sigma^r(t,t') = \Sigma^r(t-t')$. The Fourier transform of Eq. (B.7.28) is then simply:

$$\Sigma^r(\epsilon) = V^\dagger g^r_0(\epsilon) V. \quad (B.7.29)$$

The difference in Eq. (B.7.27) then becomes:

$$\frac{\Sigma^r(\epsilon + n\Omega) - \Sigma^r(\epsilon + n\Omega)^\dagger}{2i} = V^\dagger \text{Im}(g^r_0(\epsilon + n\Omega) V) = -\pi V^\dagger \sum_{\alpha \in L,R} \delta(\epsilon_\alpha - (\epsilon + n\Omega)) |\alpha\rangle \langle \alpha| V \quad (B.7.30)$$

$$= -\pi \sum_{\alpha \in L,R} \langle m|V|\alpha\rangle \delta(\epsilon_\alpha - (\epsilon + n\Omega)) \langle m|V|\alpha\rangle \quad (B.7.31)$$

$$= -\pi \sum_{\alpha \in L,R} \langle m|V|\alpha\rangle \delta(\epsilon_\alpha - (\epsilon + n\Omega)) \rho_\alpha \quad (B.7.32)$$

$$= -\frac{1}{2} \sum_{\alpha \in L,R} \sum_{m,l} \Gamma_{ml}(\epsilon + n\Omega) = -\frac{1}{2} \sum_{\alpha \in L,R} \Gamma_\alpha(\epsilon + n\Omega). \quad (B.7.34)$$

We can now insert this into Eq. (B.7.27) to get:

$$\langle J^r_L(t) \rangle = \frac{e}{\hbar} \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} d\epsilon \left[ \text{Tr} \left[ (G^{(n)}(\epsilon))^\dagger \Gamma_L(\epsilon + n\Omega) G^{(n)}(\epsilon) \Gamma_L(\epsilon) \right] f_L(\epsilon) \right] + \text{Tr} \left[ (G^{(n)}(\epsilon))^\dagger \Gamma_R(\epsilon + n\Omega) G^{(n)}(\epsilon) \Gamma_L(\epsilon) \right] f_L(\epsilon) \quad (B.7.35)$$

We now define the transmission probability:

$$T^{(n)}_{\alpha\alpha'}(\epsilon) = \text{Tr} \left[ (G^{(n)}(\epsilon))^\dagger \Gamma_\alpha(\epsilon + n\Omega) G^{(n)}(\epsilon) \Gamma_{\alpha'}(\epsilon) \right]. \quad (B.7.36)$$

The current in Eq. (B.7.35) may then be written as:

$$\langle J^r_L(t) \rangle = \frac{e}{\hbar} \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} d\epsilon \left( T^{(n)}_{RL}(\epsilon) f_L(\epsilon) + T^{(n)}_{LR}(\epsilon) f_L(\epsilon) \right). \quad (B.7.37)$$
In order to evaluate the second term in Eq. (B.7.9) we first need to find an expression for $G^<(t, t')$ this is done in Appendix (B.6). The result is:

$$G^<(t, t') = \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 G^r(t, t_1) \Sigma^<(t_1, t_2) G^a(t_2, t').$$

(B.7.38)

We have to keep in mind that we absorbed the Heaviside step function into the Fourier transform in Eq. (B.7.3). Therefore if we included the Heaviside step function Eq. (B.7.38) reads:

$$\theta(t-t')G^<(t, t') = \theta(t-t') \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 G^r(t, t_1) \Sigma^<(t_1, t_2) G^a(t_2, t').$$

(B.7.39)

The retarded and advanced Green’s functions carry the implicit Heaviside step functions $\theta(t - t_1)$ and $\theta(t_2 - t')$. Therefore the expression in Eq. (B.7.39) contains the product of 3 Heaviside functions. This product can be rewritten in the following way: $\theta(t - t')\theta(t - t_1)\theta(t_1 - t_2)\theta(t_1 - t_2)\theta(t_2 - t')$. The right hand-side is more useful when we wish to find the Fourier transform of Eq. (B.7.39). We may then write Eq. (B.7.39) as:

$$\theta(t-t')G^<(t, t') = \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 G^r(t, t_1) \Sigma^<(t_1, t_2) G^a(t_2, t'),$$

(B.7.40)

where:

$$\Sigma^<(t_1, t_2) = \theta(t_1 - t_2)\Sigma^<(t_1, t_2).$$

(B.7.41)

The Fourier transform of Eq. (B.7.40) then becomes:

$$G^<(t, \mathcal{E}) = \int_{-\infty}^{\infty} dt' \theta(t-t')G^<(t, t')e^{-i\mathcal{E}(t'-t)}$$

$$= \int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt' G^r(t, t_1) \tilde{\Sigma}^<(t_1 - t_2) G^a(t_2, t')e^{-i\mathcal{E}(t'-t)}. $$

(B.7.42)

We now use the identity $G^a(t, t') = (G^r(t', t))^\dagger$ and express the Green’s functions and the self energies in Eq. (B.7.40) in terms of the their inverse Fourier transform:

$$G^<(t, \mathcal{E}) = \frac{1}{(2\pi)^3} \sum_{n, m} \int_{-\infty}^{\infty} dE_1 \int_{-\infty}^{\infty} dE_2 \int_{-\infty}^{\infty} dE_3 \int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt' G^r(n, E_1) \tilde{\Sigma}^<(E_2) (G^r(m, E_3))^\dagger$$

$$\times e^{-i\mathcal{E}(t'-t)}e^{-iE_1(t-t_1)}e^{-iE_2(t_1-t_2)}e^{iE_3(t_2-t')}. $$

(B.7.43)

expressing the Green’s functions in terms of Floquet components we get:

$$G^<(t, \mathcal{E}) = \frac{1}{(2\pi)^3} \sum_{n, m} \int_{-\infty}^{\infty} dE_1 \int_{-\infty}^{\infty} dE_2 \int_{-\infty}^{\infty} dE_3 \int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt' G^r(n, E_1) \tilde{\Sigma}^<(E_2) (G^r(m, E_3))^\dagger$$

$$\times e^{-i\mathcal{E}(t'-t)}e^{-iE_1(t-t_1)}e^{-iE_2(t_1-t_2)}e^{iE_3(t_2-t')e^{-in\Omega t}}e^{im\Omega t'}. $$

(B.7.44)

We now rearrange the exponential functions to get

$$G^<(t, \mathcal{E}) = \frac{1}{(2\pi)^3} \sum_{n, m} \int_{-\infty}^{\infty} dE_1 \int_{-\infty}^{\infty} dE_2 \int_{-\infty}^{\infty} dE_3 \int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt' G^r(n, E_1) \tilde{\Sigma}^<(E_2) (G^r(m, E_3))^\dagger$$

$$\times e^{i(E_3 - E + m\Omega t')} e^{i(E_1 - E_2 - n\Omega t)} e^{i(E_1 - E_2 - t_1)} e^{i(E_2 - E_3 - t_2)}$$

(B.7.45)

Carrying out the time integrals is now straightforward since they are just delta functions

$$G^<(t, \mathcal{E}) = \sum_{n, m} \int_{-\infty}^{\infty} dE_1 \int_{-\infty}^{\infty} dE_2 \int_{-\infty}^{\infty} dE_3 G^r(n, E_1) \tilde{\Sigma}^<(E_2) (G^r(m, E_3))^\dagger$$

$$\times \delta(E_3 - E + m\Omega)\delta(E_1 - E_2)\delta(E_2 - E_3)e^{i(E_1 - E_2)}.$$ 

(B.7.46)

$$= \sum_{n, m} G^r(n, E - m\Omega)\tilde{\Sigma}^<(E - m\Omega) (G^r(m, E - m\Omega))^\dagger e^{i(m-n)\Omega t}.$$

(B.7.47)
Finally we calculate the time average over the lesser Green’s function:

\[
\frac{1}{T} \int_0^T \frac{d\tau}{\hbar} G^<(\tau, \mathcal{E}) = \sum_{n=-\infty}^{\infty} G^{(n)}(\mathcal{E} - n\Omega) \tilde{\Sigma}^<(\mathcal{E} - n\Omega) \left( G^{(n)}(\mathcal{E} - n\Omega) \right)^\dagger. \tag{B.7.48}
\]

The second term in the current in Eq. (B.7.9) may then be written as:

\[
\langle J^2_L(t) \rangle = -\frac{2e}{\hbar} \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} d\mathcal{E} \text{Tr} \left[ \left( G^{(n)}(\mathcal{E} - n\Omega) \right) \left( \frac{\Sigma^<(\mathcal{E} - n\Omega) - (\Sigma^<(\mathcal{E} - n\Omega))^\dagger}{2i} \right) \times (G^{(n)}(\mathcal{E} - n\Omega))^\dagger \Gamma_L(\mathcal{E}) \right]. \tag{B.7.49}
\]

In Appendix B.6 the lesser self energy is found to be:

\[
\Sigma^<(t, t') = V^\dagger g_0^<(t, t') V. \tag{B.7.52}
\]

We now apply an argument similar to that for \( \tilde{g}_0^<(t, t') \). Since \( g_0^<(t, t') = g_0^<(t - t') \), it follows from Eq. (B.7.52) that \( \Sigma^<(t, t') = \Sigma^<(t - t') \). Using Eq. (B.7.41) we then obtain:

\[
\Sigma^<(t - t') = V^\dagger \theta(t - t') g_0^<(t - t') V = \sum_\alpha V^\dagger \theta(t - t') e^{-i\epsilon_\alpha(t-t')} V f(\epsilon_\alpha). \tag{B.7.53}
\]

We are only interested in the anti-Hermitian part of the lesser self energy and its Fourier transform is

\[
\tilde{\Sigma}^<(\mathcal{E}) = (\tilde{\Sigma}^<(\mathcal{E}))^\dagger = \pi \sum_{\alpha \in L, R} V^\dagger \delta(\epsilon_\alpha - \mathcal{E}) |\alpha\rangle \langle \alpha| V f(\epsilon_\alpha) = \pi \sum_{\alpha \in L, R} \sum_{n,m} (V^\dagger)_m n \delta(\epsilon_\alpha - \mathcal{E})(V)_n f(\epsilon_\alpha) \tag{B.7.54}
\]

\[
= \pi \sum_{\alpha \in L, R} \sum_{m,n} (V(\epsilon_\alpha)^\dagger)_m n \delta(\epsilon_\alpha - \mathcal{E})(V)_n f(\epsilon_\alpha) = \pi \sum_{\alpha \in L, R} \sum_{m,n} ((V(\mathcal{E}))^\dagger)_m n \delta(\epsilon_\alpha - \mathcal{E})(V(\mathcal{E}))_n f(\epsilon_\alpha) \tag{B.7.55}
\]

\[
= \pi \sum_{m,n} \sum_{\alpha \in L, R} \sum_{\alpha \in L, R} \sum_{m,n} \Gamma_{\alpha m n}(\mathcal{E}) f(\epsilon_\alpha) = \pi \sum_{\alpha \in L, R} \sum_{m,n} \sum_{m,n} \Gamma_{\alpha m n}(\mathcal{E}) f(\epsilon_\alpha) \tag{B.7.56}
\]

The current in Eq. (B.7.51) can then be written as:

\[
\langle J^2_L(t) \rangle = -\frac{e}{\hbar} \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} d\mathcal{E} \left( \text{Tr} \left[ \left( G^{(n)}(\mathcal{E}) \right)^\dagger \Gamma_L(\mathcal{E} + n\Omega) G^{(n)}(\mathcal{E}) \right] f_L(\mathcal{E}) \right)
\]

\[
+ \text{Tr} \left[ \left( G^{(n)}(\mathcal{E}) \right)^\dagger \Gamma_L(\mathcal{E} + n\Omega) G^{(n)}(\mathcal{E}) \right] f_L(\mathcal{E}) \tag{B.7.58}
\]

In terms of the transmission probabilities defined in Eq. (B.7.36) and relabeling \( \mathcal{E}' \) as \( \mathcal{E} \) we can write the current in Eq. (B.7.58) as:

\[
\langle J^2_L(t) \rangle = -\frac{e}{\hbar} \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} d\mathcal{E} \left( T^{(n)}_L(\mathcal{E}) f_L(\mathcal{E}) + T^{(n)}_R(\mathcal{E}) f_R(\mathcal{E}) \right). \tag{B.7.59}
\]
We can now finally find the total current through the system in Eq. (B.7.9) by adding up the contributions in Eq. (B.7.37) and Eq. (B.7.59) to get:

\[ \langle J_L(t) \rangle = \frac{e}{h} \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} d\epsilon \left( T_{RL}^{(n)}(\epsilon) f_L(\epsilon) - T_{LR}^{(n)}(\epsilon) f_R(\epsilon) \right). \]  

(B.7.60)

**B.8 Expression for the time-averaged density \( n_i \)**

The time-averaged local particle density is defined as:

\[ \langle \langle n_i(t) \rangle \rangle = \frac{1}{T} \int_0^T dt \langle n_i(t) \rangle = \frac{1}{T} \int_0^T dt \langle c_i^\dagger(t) c_i(t) \rangle = \frac{-i}{T} \int_0^T dt G_{i,i}^{-}(t,t) \]  

(B.8.1)

In Appendix B.6 we obtained an expression for the lesser Greens function \( G^{-}(t, t') \). At equal times it reads:

\[ G^{-}(t, t) = \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 G^r(t, t_1) \Sigma^{-}(t_1, t_2) G^a(t_2, t). \]  

(B.8.2)

We now use the identity \( G^a(t', t) = (G^r(t', t))^\dagger \) to write Eq. B.8.2 as:

\[ G^{-}(t, t) = \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 G^r(t, t_1) \Sigma^{-}(t_1, t_2) (G^r(t, t_2))^\dagger \]  

(B.8.3)

We now express the retarded Green’s functions as well as the lesser self energy in terms of their inverse Fourier transforms:

\[ G^{-}(t, t) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{\infty} d\epsilon \int_{-\infty}^{\infty} d\epsilon_1 \int_{-\infty}^{\infty} d\epsilon_2 G^r(t, \epsilon) \Sigma^{-}(\epsilon_1) (G^r(t, \epsilon_2))^\dagger \times e^{-i\epsilon(t-t_1)} e^{-i\epsilon_1(t_1-t_2)} e^{i\epsilon_2(t-2-t_2)} \]  

(B.8.4)

We can now decompose the Green’s functions into Floquet Green’s functions to get:

\[ G^{-}(t, t) = \frac{1}{(2\pi)^3} \sum_{m, n=-\infty}^{\infty} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{\infty} d\epsilon \int_{-\infty}^{\infty} d\epsilon_1 \int_{-\infty}^{\infty} d\epsilon_2 \times G^{r(n)}(\epsilon) \Sigma^{-}(\epsilon_1) (G^{r(m)}(\epsilon_2))^\dagger \times e^{-i\epsilon(t-t_1)} e^{-i\epsilon_1(t_1-t_2)} e^{i\epsilon_2(t-2-t_2)} \times G^{r(n)}(\epsilon) \Sigma^{-}(\epsilon_1) (G^{r(m)}(\epsilon_2))^\dagger \]  

(B.8.5)

The time averaged lesser Green’s function is then:

\[ \frac{1}{T} \int_0^T dt G^{-}(t, t) = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} d\epsilon G^{r(n)}(\epsilon) \Sigma^{-}(\epsilon) (G^{r(n)}(\epsilon))^\dagger \]  

(B.8.6)

The time-averaged local particle density then becomes:

\[ \langle \langle n_i(t) \rangle \rangle = \frac{-i}{2\pi} \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} d\epsilon \left( G^{r(n)}(\epsilon) \Sigma^{-}(\epsilon) (G^{r(n)}(\epsilon))^\dagger \right)_{i,i} \]  

(B.8.7)
Using the result from Eq. (B.6.22) in Appendix B.6 we know that the lesser self energy is given by:

$$\Sigma^<(t, t') = V^\dagger g^<(t, t') V$$  \hspace{1cm} (B.8.8)

Using the expression for the bare lesser Green’s function in Eq. 4.2.2 we have obtain the lesser self energy in the energy domain:

$$\Sigma^<(\epsilon) = \sum_{m,n,\alpha \in L,R} \left( V^\dagger \right)_{m,\alpha} i f(\epsilon_n) \int_{-\infty}^{\infty} dt (t-t') \left( e^{i\epsilon_n(t-t')} e^{-i\epsilon(t-t')} \right) V_{\alpha,n}$$

$$= \sum_{m,n,\alpha \in L,R} \left( V^\dagger \right)_{m,\alpha} i f(\epsilon_n) 2\pi \delta(\epsilon_n - \epsilon) V_{\alpha,n}$$

$$= \sum_{\alpha \in L,R} f_{\alpha} \sum_{m,n} \left( V(\epsilon_n)^\dagger \right)_{m} i f_{\alpha} 2\pi \delta(\epsilon_n - \epsilon) V(\epsilon_n)_n$$

$$i 2\pi \sum_{m,n,\alpha \in L,R} \left( V(\epsilon_n)^\dagger \right)_{m} f_{\alpha} \delta(\epsilon_n - \epsilon) V(\epsilon_n)_n = \sum_{\alpha \in L,R} f_{\alpha} \left( \Gamma_{\alpha}(\epsilon) = i (f_{L}(\epsilon) \Gamma_{L}(\epsilon) + f_{R}(\epsilon) \Gamma_{R}(\epsilon)) \right)$$  \hspace{1cm} (B.8.9)

Inserting this expression for the lesser self energy into Eq. (B.8.7) we obtain:

$$\langle \langle n_{i}(t) \rangle \rangle = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} \epsilon \left[ f_{L}(\epsilon) \left( G^{(n)}(\epsilon) \Gamma_{L}(\epsilon) \left( G^{(n)}(\epsilon) \right)^\dagger \right) \right]_{i,i} +$$

$$f_{R}(\epsilon) \left( G^{(n)}(\epsilon) \Gamma_{R}(\epsilon) \left( G^{(n)}(\epsilon) \right)^\dagger \right)_{i,i} \right].$$  \hspace{1cm} (B.8.10)

Now we write out the matrix product in Eq. (B.8.10)

$$\langle \langle n_{i}(t) \rangle \rangle = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} \epsilon \left[ f_{L}(\epsilon) \left| G^{(n)}(\epsilon) \right|^{2} (\Gamma_{L}(\epsilon))_{k,k} + f_{R}(\epsilon) \left| G^{(n)}(\epsilon) \right|^{2} (\Gamma_{R}(\epsilon))_{k,k} \right].$$  \hspace{1cm} (B.8.11)

The expression for the density in Eq. (B.8.11) simplifies further since we are working in the wide-band limit where \( \Gamma_{L/R}(\epsilon) = \Gamma_{L/R} \). We then obtain our final expression for the density:

$$\langle \langle n_{i}(t) \rangle \rangle = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} \epsilon \left[ f_{L}(\epsilon) \left| G^{(n)}(\epsilon) \right|^{2} (\Gamma_{L})_{k,k} + f_{R}(\epsilon) \left| G^{(n)}(\epsilon) \right|^{2} (\Gamma_{R})_{k,k} \right].$$  \hspace{1cm} (B.8.12)

### B.9 Expression for the time averaged current density \( j_{ij} \)

In this appendix we set out to find an expression for the time-averaged current density. For the graphene Hamiltonian the magnetic vector potential is \( A_{ij}(t) = \frac{\epsilon}{\hbar} (A(t))_{ij} = (-\frac{\epsilon}{\hbar}) A(t) \cdot (r_j - r_i) \). The current operator can be obtained from a Hamiltonian using the following expression [37, 42]:

$$j_{ij}(t) = \frac{\delta H}{\delta (A(t))_{ij}};$$  \hspace{1cm} (B.9.1)

where \( \frac{\delta}{\delta (A(t))_{ij}} \) denotes the functional derivative with respect to \( (A(t))_{ij} = A(t) \cdot (r_j - r_i) \). Using the graphene Hamiltonian defined in Eq. (3.3.1) in the main text we get

$$j_{ij}(t) = -\frac{\epsilon}{\hbar} \left( i J_{ij}(t) c_i^\dagger c_j + i (J_{ij}(t))^* c_j^\dagger c_i \right);$$  \hspace{1cm} (B.9.2)

taking the expectation value and the time average over one period we get:

$$\langle \langle j_{ij}(t) \rangle \rangle = -\frac{e}{\hbar} \frac{1}{T} \int_{0}^{T} dt \left( J_{ij}(t) G_{ij}^\dagger(t,t) + (J_{ij}(t))^* (G_{ij}^\dagger(t,t))^* \right) = -\frac{e}{\hbar} \frac{1}{T} \int_{0}^{T} dt 2\text{Re} \left( J_{ij}(t) G_{ij}^\dagger(t,t) \right).$$  \hspace{1cm} (B.9.3)
We can apply the result we obtained for $G^<(t,t)$ in Appendix B.8 to write the bonding current as

$$
\langle \langle j_{ij}(t) \rangle \rangle = -\frac{e}{\hbar} \frac{2}{2\pi} \text{Re} \left[ \sum_{m,n,-\infty}^{\infty} \int_{-\infty}^{\infty} d\mathcal{E} \left( G^{(r)}(\mathcal{E}) \Sigma^<(\mathcal{E}) \left( G^{(m)}(\mathcal{E}) \right)^\dagger \right) \frac{J_1}{T} \int_{0}^{T} dt e^{i(m-n)\Omega t} e^{iA_{ij}(t)} \right]
$$

(B.9.4)

For the $ij$th bond we have $A_{ij}(t) = \frac{\alpha e A}{h} \cos(\phi_{ij} - \rho \Omega t)$. By applying the Jacobi-Anger expansion introduced in Eq. (A.6.6) we obtain

$$
\langle \langle j_{ij}(t) \rangle \rangle = -\frac{e}{\hbar} \frac{2}{2\pi} \text{Re} \left[ \sum_{m,n,-\infty}^{\infty} \int_{-\infty}^{\infty} d\mathcal{E} \left( G^{(r)}(\mathcal{E}) \Sigma^<(\mathcal{E}) \left( G^{(m)}(\mathcal{E}) \right)^\dagger \right) \frac{J_1}{T} \int_{0}^{T} dt e^{i(m-n)\Omega t} \mathcal{J}_L(\lambda) e^{i\lambda(t-\rho \Omega t)} \right]
$$

(B.9.5)

$$
\langle \langle j_{ij}(t) \rangle \rangle = -\frac{e}{\hbar} \frac{2}{2\pi} \sum_{m,n,-\infty}^{\infty} \int_{-\infty}^{\infty} d\mathcal{E} \text{Re} \left[ \left( G^{(r)}(\mathcal{E}) \Sigma^<(\mathcal{E}) \left( G^{(m)}(\mathcal{E}) \right)^\dagger \right) \frac{J_1}{T} \int_{0}^{T} dt e^{i(m-n)\Omega t} \mathcal{J}_R(\lambda) e^{i\phi_{ij}(t-\rho \Omega t)} \right]
$$

(B.9.6)

where $J_{\rho(m-n)}(\lambda) = J_1 \mathcal{J}_{\rho(m-n)}(\lambda)$. In Appendix B.8 we obtained an expression for $\Sigma^<(\mathcal{E})$. By inserting this result and taking the wide band limit we get:

$$
\langle \langle j_{ij}(t) \rangle \rangle = \frac{2e}{\hbar} \sum_{m,n,-\infty}^{\infty} \int_{-\infty}^{\infty} d\mathcal{E} \text{Im} \left[ \left( G^{(r)}(\mathcal{E}) \Gamma_L \left( G^{(m)}(\mathcal{E}) \right)^\dagger \right) \frac{J_1}{T} \int_{0}^{T} dt e^{i\phi_{ij}(t-\rho \Omega t)} \right]
$$

$$
-\frac{2e}{\hbar} \sum_{m,n,-\infty}^{\infty} \int_{-\infty}^{\infty} d\mathcal{E} \text{Re} \left[ \left( G^{(r)}(\mathcal{E}) \Gamma_R \left( G^{(m)}(\mathcal{E}) \right)^\dagger \right) \frac{J_1}{T} \int_{0}^{T} dt e^{i\phi_{ij}(t-\rho \Omega t)} \right]
$$

(B.9.7)

where we used $\text{Re}(iz) = -\text{Im}(z)$.

### B.10 Expression for the non-equilibrium distribution function

We are interested in the following quantity

$$
G^{<0}(\mathcal{E}) = \frac{1}{T} \int_{0}^{T} dt G^{<}(t,\mathcal{E}) = \frac{1}{T} \int_{0}^{T} dt \int_{-\infty}^{\infty} dt' e^{i\mathcal{E}(t-t')} G^{<}(t,t')
$$

(B.10.1)

Previously we obtained an expression for the lesser Green’s function

$$
G^<(t,t') = \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 G^r(t,t_1) \Sigma^<(t_1,t_2) G^m(t_2,t').
$$

(B.10.2)

We now use the identity $G^r(t,t') = (G^r(t',t))^\dagger$ to write the lesser Green’s function as

$$
G^<(t,t') = \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 G^r(t,t_1) \Sigma^<(t_1,t_2) (G^r(t',t_2))^\dagger
$$

(B.10.3)

We now express the retarded Green’s functions as well as the lesser self energy in terms of their inverse Fourier transforms:

$$
G^<(t,t') = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{\infty} d\mathcal{E}_1 \int_{-\infty}^{\infty} d\mathcal{E}_2 \int_{-\infty}^{\infty} d\mathcal{E}_3 G^r(t,\mathcal{E}) \Sigma^<(\mathcal{E}_1) (G^r(t,\mathcal{E}_2))^\dagger \times e^{-i\mathcal{E}_1(t-t_1)} e^{-i\mathcal{E}_2(t_1-t_2)} e^{i\mathcal{E}_3(t'-t_2)}
$$

(B.10.4)
We can now decompose the retarded Green’s functions into Floquet Green’s functions. The lesser Green’s function introduced in Eq. (B.10.1):

We now take the Fourier transform and perform a time average on both sides of Eq. (B.10.5) to get the

Hence we may write

\[
G^< (t, t') = \frac{1}{(2\pi)^3} \sum_{m,n=\ldots}^{\infty} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{\infty} dE \int_{-\infty}^{\infty} d\epsilon_1 \int_{-\infty}^{\infty} d\epsilon_2 
\times G^{r(n)} (E) \Sigma^< (E_1) \left( G^{r(m)} (E_2) \right) ^\dagger \times e^{-iE(t-t_1)} e^{-iE_1(t_1-t_2)} e^{iE_2(t_2-t')} e^{i\epsilon \Omega t} e^{-i\epsilon \Omega t}
\]

\[
= \frac{1}{(2\pi)^3} \sum_{m,n=\ldots}^{\infty} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{\infty} dE \int_{-\infty}^{\infty} d\epsilon_1 \int_{-\infty}^{\infty} d\epsilon_2 
\times G^{r(n)} (E) \Sigma^< (E_1) \left( G^{r(m)} (E_2) \right) ^\dagger \times e^{i(E-E_1)t_1} e^{i(E_1-E_2)t_2} e^{iE_2(t_2-t')} e^{-i(E+n\Omega)t}
\]

\[
= \frac{1}{2\pi} \sum_{m,n=\ldots}^{\infty} \int_{-\infty}^{\infty} d\epsilon_2 G^{r(n)} (E_2) \Sigma^< (E_2) \left( G^{r(m)} (E_2) \right) ^\dagger \times e^{iE_2+n\Omega \epsilon} e^{-i(E_2+n\Omega)\epsilon}.
\] (B.10.5)

We now take the Fourier transform and perform a time average on both sides of Eq. (B.10.5) to get the lesser Green’s function introduced in Eq. (B.10.1):

\[
G^{< (0)} (E) = \frac{1}{2\pi} \sum_{m,n=\ldots}^{\infty} \int_{-\infty}^{\infty} dE_2 \frac{1}{T} \int_{0}^{T} dt \int_{-\infty}^{\infty} d\epsilon \int_{-\infty}^{\infty} d\epsilon' e^{iE(t-t')} G^{r(n)} (E_2) \Sigma^< (E_2) \left( G^{r(m)} (E_2) \right) ^\dagger 
\times e^{i(E_2+n\Omega \epsilon)} e^{-i(E_2+n\Omega)\epsilon}
\]

\[
= \sum_{m,n=\ldots}^{\infty} \frac{1}{T} \int_{0}^{T} dt e^{iE_2 \epsilon} \int_{-\infty}^{\infty} dE_2 G^{r(n)} (E_2) \Sigma^< (E_2) \left( G^{r(m)} (E_2) \right) ^\dagger \frac{1}{2\pi} \int_{-\infty}^{\infty} dt' e^{iE_2 \epsilon - \epsilon'}
\]

\[
= \sum_{m,n=\ldots}^{\infty} \frac{1}{T} \int_{0}^{T} dt G^{r(n)} (E - m\Omega) \Sigma^< (E - m\Omega) \left( G^{r(m)} (E - m\Omega) \right) ^\dagger e^{i(m-n)\Omega t}
\]

\[
= \sum_{n=\ldots}^{\infty} G^{r(n)} (E - n\Omega) \Sigma^< (E - n\Omega) \left( G^{r(n)} (E - n\Omega) \right) ^\dagger
\] (B.10.6)

In Appendix B.8 we found the lesser self energy

\[
\Sigma^< (E) = i \left( f_L (E) \Gamma_L (E) + f_R (E) \Gamma_R (E) \right)
\] (B.10.7)

Hence we may write

\[
G^{< (0)} (E) = i \sum_{n=\ldots}^{\infty} \left( G^{r(n)} (E - n\Omega) f_L (E - n\Omega) \Gamma_L (E - n\Omega) \left( G^{r(n)} (E - n\Omega) \right) ^\dagger 
+ G^{r(n)} (E - n\Omega) f_R (E - n\Omega) \Gamma_R (E - n\Omega) \left( G^{r(n)} (E - n\Omega) \right) ^\dagger \right)
\] (B.10.8)

In the wide band limit

\[
G^{< (0)} (E) = i \sum_{n=\ldots}^{\infty} \left( G^{r(n)} (E - n\Omega) \Gamma_L \left( G^{r(n)} (E - n\Omega) \right) ^\dagger f_L (E - n\Omega) 
+ G^{r(n)} (E - n\Omega) \Gamma_R \left( G^{r(n)} (E - n\Omega) \right) ^\dagger f_R (E - n\Omega) \right)
\] (B.10.9)
Taking the imaginary part and the trace we get:

$$\text{Im} \left( G^{\leq(0)}(\mathcal{E}) \right) = \sum_{n=-\infty}^{\infty} \left( G^{r(n)}(\mathcal{E} - n\Omega) \Gamma_L \left( G^{r(n)}(\mathcal{E} - n\Omega) \right)^\dagger f_L(\mathcal{E} - n\Omega) \right) + G^{r(n)}(\mathcal{E} - n\Omega) \Gamma_R \left( G^{r(n)}(\mathcal{E} - n\Omega) \right)^\dagger f_R(\mathcal{E} - n\Omega)$$

(B.10.10)

For an equilibrium non-interacting system the lesser Green’s function is simply:

$$g^{\leq}(\mathcal{E}) = i2\pi\rho(\mathcal{E}) f(\mathcal{E})$$

(B.10.11)

So we need to take the imaginary part and divide by the density of states as well as $2\pi$ to get the distribution function. We expect that by doing the same thing to $G^{(0)}(\mathcal{E})$ we obtain the non-equilibrium distribution function.
Appendix C

Derivations for Chapter 6

C.1 Driven finite graphene sheet with nearest neighbor hopping

We now turn our attention to finite graphene sheet under the influence of circularly polarized light. The Hamiltonian is

$$H = \sum_{\langle ij \rangle} \left( J_1 e^{iA_{ij}(t)} c_i^\dagger c_j + \text{h.c.} \right),$$

(C.1.1)

where:

$$A_{ij}(t) = \frac{e}{\hbar} A(t) \cdot (r_j - r_i), \quad A(t) = A(\cos(\Omega t), \rho \sin(\Omega t)),\)$$

(C.1.2)

Here $\rho = \pm 1$ and indicates the handedness of the circular drive. To analyze the system we need to find the Fourier coefficients so that we can apply the extended space formalism. The coefficients are given by:

$$H_n = \sum_{\langle ij \rangle} \left( c_i^\dagger c_j \left[ \frac{J_1}{T} \int_0^T dt e^{iA_{ij}(t)} e^{-i n \Omega t} \right] + c_j^\dagger c_i \left[ \frac{J_1}{T} \int_0^T dt e^{-iA_{ij}(t)} e^{-i n \Omega t} \right] \right)$$

(C.1.3)

For the $ij$’th bond we have $A_{ij}(t) = \frac{a e A}{\hbar} \cos(\phi_{ij} - \rho \Omega t)$. Using the Jacobi-Anger expansion we get:

$$H_n = \sum_{\langle ij \rangle} \sum_{l=-\infty}^{\infty} \left( c_i^\dagger c_j \left[ \frac{J_1}{T} \int_0^T dt e^{-i n \Omega t} i^l J_l(\lambda) e^{i l (\phi_{ij} - \rho \Omega t)} \right] + c_j^\dagger c_i \left[ \frac{J_1}{T} \int_0^T dt e^{-i n \Omega t} i^l J_l(\lambda) e^{-i l (\phi_{ij} - \rho \Omega t)} \right] \right)$$

$$H_n = \sum_{\langle ij \rangle} \left( c_i^\dagger c_j \left[ J_{-\rho n}(\lambda) e^{-i n \Omega t (\hat{\xi} + \phi_{ij})} \right] + c_j^\dagger c_i \left[ J_{\rho n}(\lambda) e^{i n \Omega t (\hat{\xi} - \phi_{ij})} \right] \right),$$

(C.1.4)

where we defined $J_{\rho n}(\lambda) = J_1 \mathcal{J}_{\rho n}(\lambda)$.

C.2 Numerical tests of the sum rule

Here we show the results of our numerical test of the sum rule presented in the main text. We have tested the sum rule in the off-resonant as well as the on-resonant case. The system and drive parameters used are the same as in those used for the figures presented in the main text. The results are showed in Fig. C.1a and C.1b.
Figure C.1: a) Values of time averaged differential conductance computed at $\mu = 0 \pm n\Omega$, where $n = 0, 1, 2$. This plot is for the off-resonant case. b) Values of time averaged differential conductance computed at $\mu = 0 \pm n\Omega$, where $n = 0, 1, 2$. This plot is for the on-resonant case.

C.3 Finite size effect of the energy filtering leads

As mentioned in the main text the filter has to be sufficiently large for quantum tunneling to be suppressed. In addition it must also be large enough that finite size effects are no longer present, such that the filter behaves like the model in Eq. 6.2.2 in the thermodynamic limit. Depicted in the figures below are close up plots of the of time-averaged differential conductance plots shown in the main text. Beside each plot is one for almost identical parameters, where the only difference is that the filter length is 50 instead of 100. We see that the plateaus are much smoother when the filter length is 100 than when it is only 50. This hints that finite size effects explain why the plateaus are not smooth as stated in the main text.

Figure C.2: a) Closeup of the differential conductance presented in Fig. 6.3a in the main text. b) The same plot as in Fig. C.2a but with a filter length $L_f = 50$. 

Figure C.3: Closeup of the differential conductance presented in Fig. 6.3b in the main text. b) The same plot as in Fig. C.3a but with a filter length $L_f = 50$. 