Quantum Oscillations in Graphene Rings

Bachelor’s Thesis in Physics

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17.7.2015
Ich versichere, dass ich die Arbeit selbständig verfasst und keine anderen als die angegebenen Quellen und Hilfsmittel benutzt sowie Zitate kenntlich gemacht habe.

Aachen, 17.7.2015
Abstract

The goal of this thesis is to understand a measured conductance trace of a graphene ring. A prominent feature that was observed resembles a step. We discuss different possible origins with computer simulations. Beginning with the effect of conductance quantization that leads to steps visible in the simulation. We argue that this kind of modulation is not present in the experimental data. Next, we study the signatures created by the classical transport properties of the system and compare the results with the experiment. We present simulation results that suggest that the observed effect is of classic nature.
ABSTRACT
## Contents

**Abstract** v

1 Introduction to graphene 1  
1.1 Graphene lattice .......................... 1  
1.2 Dispersion relation ......................... 2  
1.3 Classical motion .......................... 6  
1.4 Landau levels ............................. 7  

2 Simulation methods 11  
2.1 Tight-binding simulation .................... 11  
2.2 Tracing of the classical trajectories .......... 13  

3 Connection to the ring 15  
3.1 Zig-zag and armchair ........................ 15  
3.2 Dispersion relation of nanoribbons .......... 15  
3.3 The influence of a magnetic field ............. 17  
3.4 Impedance matching ........................ 20  
3.5 T-Junction .................................. 22  

4 Transport through a graphene ring 25  
4.1 Experimental data ........................... 25  
4.2 Increase of conductivity ..................... 27  
4.3 Conductance quantization ..................... 28  
4.4 Signatures of ballistic transport .............. 29  
4.5 Aharonov-Bohm oscillations .................. 35  

5 Summary 39  

Bibliography 41
Chapter 1

Introduction to graphene

Graphene is a two dimensional carbon material that is organized in a honeycomb lattice shown in Fig. 1.1. Graphene was long thought to be thermodynamically instable at any finite temperature [1]. Thus, it was a major break-through when Andre Geim and Kostaya Novoselov demonstrated that it can be produced by exfoliation which was awarded with the Nobel-prize in physics. Exfoliation is a method that removes just a few layers of graphite and sequentially reduce the numbers of layer until only one layer of graphene remains [2]. Graphene can therefore be viewed as mono-layer graphite.

1.1 Graphene lattice

A single carbon atom has the electron configuration \([\text{He}]^2s^22p^2\). In graphene, one \(s\) orbital and two \(p\) orbitals hybridize to form three \(sp^2\) orbitals. These form \(\sigma\)-bonds to the three direct neighbors. These bonds have a length of 1.42 Å and are responsible for the extraordinary mechanical properties of graphene. The remaining \(p_z\) orbital is orientated orthogonal to the graphene surface and forms the \(\pi\)-band. It is half filled and therefore exhibits conductive properties [3].

The graphene honeycomb lattice is spanned by the lattice vectors

\[
\mathbf{a}_1 = a \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \mathbf{a}_2 = \frac{a}{2} \begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix}
\]

where \(a \approx 2.46\,\text{Å}\) is the lattice constant. The lattice has two carbon atoms in its basis located at

\[
\mathbf{r}_A = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \text{and} \quad \mathbf{r}_B = \frac{a}{\sqrt{3}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}.
\]

The part of the lattice that is made up from atoms which are on sites equivalent to \(\mathbf{r}_A\) is called sublattice \(A\). The counterpart from sites equivalent to \(\mathbf{r}_B\) is called sublattice \(B\). We show the graphene lattice in Fig. 1.1.

Both sublattices are equal in a sense that they are exchangeable under the reflection symmetry

\[
A \leftrightarrow B, \quad \mathbf{r} \mapsto \mathbf{r}_B + \begin{pmatrix} \mathbf{r}_x \\ -\mathbf{r}_y \end{pmatrix}
\]
and under the rotational symmetry
\[ A \leftrightarrow B, \quad r \mapsto R_\alpha (r - r_B) \]  
(1.4)
in which \( R_\alpha \) denotes a rotation matrix by the angle \( \alpha \). Additional the honeycomb lattice is invariant under rotations about \( 2\pi/3 \).

The vectors \( b_i \) that span the reciprocal lattice of graphene are given by the relation \( a_i \cdot b_j = 2\pi \delta_{ij} \) and are found to be
\[ b_1 = \frac{2\pi}{\sqrt{3}a} \begin{pmatrix} \sqrt{3} \\ -1 \end{pmatrix} \quad \text{and} \quad b_2 = \frac{2\pi}{\sqrt{3}a} \begin{pmatrix} 0 \\ 2 \end{pmatrix}. \]  
(1.5)

1.2 Dispersion relation

The electronic structure that is responsible for the conductivity can be understood in a tight-binding picture in which only the \( p_z \)-orbitals of the carbon atoms take part [3]. In the nearest neighbor approximation only the hopping amplitude \( t \) to the three nearest neighbors is finite and must be equal for both sublattices because of the lattice symmetries. Also the onsite term on both sublattices must be equal and both can be chosen to be 0. \[ \] The tight-binding

\[ \]
1.2. DISPERSION RELATION

![Figure 1.2: Plot of the reciprocal lattice of graphene. We show the reciprocal lattice vectors $b_1$ and $b_2$ and the Wigner-Seitz unit cell. The $K$ and $K'$ points and those that are equivalent to them are shown.](image)

Hamiltonian of bulk graphene is given by

$$H = -t \begin{pmatrix} 0 & f^*(k) \\ f(k) & 0 \end{pmatrix} \quad \text{with} \quad f(k) = e^{-i\frac{\pi}{\sqrt{3}}k_y} + 2\cos\left(\frac{a}{2}k_x\right)e^{i\frac{\pi}{\sqrt{3}}k_y} \quad (1.6)$$

as derived in [4]. It operates on a two component wave function

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}, \quad (1.7)$$

that contains the probability amplitude for the $A$ and $B$ sublattice. $\psi$ is element of the product space $\mathcal{H}_k \otimes \mathcal{H}_{sz}$, where $\mathcal{H}_k$ is the two dimensional momentum space and $\mathcal{H}_{sz}$ contains the two states $|\uparrow\rangle$ and $|\downarrow\rangle$. $\mathcal{H}_{sz}$ is called the pseudo spin space in which $|\uparrow\rangle$ means polarization on the sublattice $A$ and $|\downarrow\rangle$ means polarization on the sublattice $B$. Because the structure of the Hamiltonian is equivalent to a spinor structure, we can bring it into the form

$$H = -t \text{Re} \left( f(k) \right) \sigma_x - t \text{Im} \left( f(k) \right) \sigma_y \quad (1.8)$$

that respects the pseudo-spin structure. The $\sigma_i$ denote the Pauli matrices that operate on the pseudo spin.

The Hamiltonian is already diagonal in the momentum space, in the pseudo spin space we can diagonalize it and find the eigenvectors

$$|\psi_+\rangle = \frac{1}{\sqrt{2}} \left( |k, \uparrow\rangle + \frac{f(k)}{|f(k)|} |k, \downarrow\rangle \right) \quad \text{and} \quad |\psi_-\rangle = \frac{1}{\sqrt{2}} \left( |k, \uparrow\rangle - \frac{f(k)}{|f(k)|} |k, \downarrow\rangle \right) \quad (1.9)$$
CHAPTER 1. INTRODUCTION TO GRAPHENE

Figure 1.3: A line cut through the band structure of graphene is presented. The $\pi^+$ and $\pi^-$ bands are shown. The two Dirac cones around the points $\mathbf{K}$ and $\mathbf{K}'$ are clearly visible. The linearization of the band structure around $\mathbf{K}'$ is indicated.

with the corresponding eigenenergies

$$E = \pm |f(\mathbf{k})| = \pm t \sqrt{1 + 4 \cos \left( \frac{a}{2} k_x \right) \cos \left( \frac{\sqrt{3} a}{2} k_y \right) + 4 \cos^2 \left( \frac{a}{2} k_x \right)}. \quad (1.10)$$

The states $|\psi_+\rangle$ all have positive energies and form the $\pi^+$-band. The states $|\psi_-\rangle$ all have negative energies and form the $\pi^-$-band.

We see that there are modes at zero energy at the points

$$\mathbf{K} = \frac{4\pi}{3a} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \mathbf{K}' = \frac{4\pi}{3a} \begin{pmatrix} -1 \\ 0 \end{pmatrix} \quad (1.11)$$

of the reciprocal lattice. The other points with zero energy are connected to $\mathbf{K}$ and $\mathbf{K}'$ by the rotational symmetry of the lattice. A line cut through the band structure is shown in Fig. 1.3. We are specially interested in the very low energy states because in graphene experiments the Fermi energy is close to zero and only states with a comparable energy have an influence on the behavior of the system. By neglecting high energy states we separate the dispersion relation in two independent domains called valleys. In one domain there are states that are close to $\mathbf{K}$ and in the other there are states that are close to $\mathbf{K}'$. We want to note this difference by introducing an additional quantum number $\xi$ that is 1 for states close to $\mathbf{K}$ and $-1$ for states that are close to $\mathbf{K}'$. Also, we want to refer to $\mathbf{K}$ as $\mathbf{K}_1$ and $\mathbf{K}'$ as $\mathbf{K}_{-1}$. To be able to treat states around $\mathbf{K}$ and $\mathbf{K}'$ simultaneous we want to shift the origin of the momentum space separately such that we only study small excitations from $\mathbf{K}_\pm$. We do it by defining the new wave vector $\mathbf{q}$ to be

$$\mathbf{q} = \mathbf{k} - \mathbf{K}_\xi \quad (1.12)$$
1.2. DISPERSION RELATION

and denote these states as

$$|q, \xi, s_z\rangle \in \mathcal{H}_q \otimes \mathcal{H}_\xi \otimes \mathcal{H}_s$$

(1.13)

where $\mathcal{H}_\xi$ is the valley space that contains the states $|\xi = \pm 1\rangle$ and $\mathcal{H}_q$ is the new momentum space with shifted origin.

Because we now study only small excitation from the Dirac points $K_\xi$, we can expand the Hamiltonian around $q = 0$ which yields

$$H_\xi = -\text{Re} \left( q \cdot \nabla f(k)|_{k = K_\xi} \right) \sigma_x - \text{Im} \left( q \cdot \nabla f(k)|_{k = K_\xi} \right) \sigma_y$$

(1.14)

$$= \frac{\sqrt{3}}{2} ta (\xi q_x \sigma_x + q_y \sigma_y)$$

(1.15)

The eigenstates of the expanded Hamiltonian are

$$|\psi_+, \xi\rangle = \frac{1}{\sqrt{2}} \left( |k, \xi, \uparrow\rangle + \frac{\xi q_x + i q_y}{|q|} |k, \xi, \downarrow\rangle \right)$$

$$|\psi_-, \xi\rangle = \frac{1}{\sqrt{2}} \left( |k, \xi, \uparrow\rangle - \frac{\xi q_x + i q_y}{|q|} |k, \xi, \downarrow\rangle \right)$$

with the corresponding eigenvalues

$$E(q) = \pm \frac{\sqrt{3}}{2} ta |q|.$$ (1.16)

We found a linear energy-momentum relation, that is called a Dirac cone.

In a next step we combine the two Hamiltonians in order to treat the two valley configurations simultaneous. The complete Hamiltonian with both Dirac cones in matrix notation has the form

$$H = \frac{\sqrt{3}}{2} ta \begin{pmatrix} q_x \sigma_x + q_y \sigma_y & 0 \\ 0 & -q_x \sigma_x + q_y \sigma_y \end{pmatrix}$$

(1.17)

and operates on a wave function

$$\psi = \begin{pmatrix} \psi_{\xi = 1} \\ \psi_{\xi = -1} \end{pmatrix}$$

(1.18)

in which both components have the form of the wave function in Eq. (1.7).

By performing the unitary transformation

$$H \rightarrow H_D = U H U^\dagger, \quad \psi \rightarrow \psi_D = U \psi, \quad U = \begin{pmatrix} \sigma_0 & 0 \\ 0 & \sigma_y \end{pmatrix}$$

(1.19)

we yield the Hamiltonian

$$H_D = \frac{\sqrt{3}}{2} ta q \cdot \sigma \text{ id}_\xi$$

(1.20)

that acts as the identity operation $\text{id}_\xi$ on the valley degree of freedom. It is important to note that by transforming the Hamiltonian into the form of a Dirac Hamiltonian, we can only stick to the sublattice polarization interpretation of $|\uparrow\rangle$ and $|\downarrow\rangle$ as long as we have a complete valley degeneracy.
The linear energy-momentum relation we obtained implies a velocity

\[ v_f = \frac{\sqrt{3}}{2\hbar} at \]  

(1.21)

that is called the Fermi velocity and can experimentally be found to be \( v_f \approx 10 \times 10^6 \text{ m s}^{-1} \). It corresponds to \( t \approx 2.8 \text{ eV} \). We can now define the momentum \( p = hq \) and give the Hamiltonian for bulk graphene

\[ H = v_f p \cdot \sigma. \]  

(1.22)

We imply the identity operation on the valley-space when we use it.

1.3 Classical motion

To understand the behavior of graphene under the influence of a magnetic field, we first study the classical behavior of the electrons in graphene. The quantum mechanically derived Hamiltonian implies the classical Hamiltonian \( H = v_f |p| \). For this problem we can solve the Hamiltonian equations of motions

\[ \frac{\partial H}{\partial x_i} = \frac{dp_i}{dt} \quad \text{and} \quad \frac{\partial H}{\partial p_i} = -\frac{dx_i}{dt}. \]  

(1.23)

To implement the magnetic field we have to perform the minimal coupling substitution

\[ p \mapsto p + eA \]  

(1.24)

for a particle of charge \(-e\) where \( A \) is the vector potential of the applied magnetic field such that \( B = \nabla \times A \). The vector potential is gauge invariant, therefore we can choose a gauge that is appropriate. For our problem we choose the Landau gauge

\[ A = -Bye_x. \]  

(1.25)

It respects the invariance of the problem under translations along the \( x \)-axis which makes the calculations easier. By performing the substitution we obtain the Hamiltonian

\[ H = v_f \sqrt{(p_x - By)^2 + p_y^2}. \]  

(1.26)

The Hamiltonian is neither dependent on the time nor is it dependent on the coordinate \( x \). Therefore, the energy \( E = H \) and the canonic momentum \( p_x \) are constants of motion. We start with solving for the motion in the \( y \)-space

\[ \frac{\partial H}{\partial p_y} = \frac{v_f^2}{H} p_y = \frac{dy}{dt}, \quad \frac{\partial H}{\partial y} = \frac{Bev_f^2}{H} (By - p_x) = -\frac{dp_y}{dt} \]  

(1.27)

and see that the motion forms a harmonic oscillator for the momenta \( p_y \)

\[ \frac{d^2 p_y}{dt^2} = -\frac{B^2 e^2 v_f^3}{H^2} \frac{dy}{dt} = -\frac{B^2 e^2 v_f^3}{H^2} p_y. \]  

(1.28)

The general solution of Eq. (1.28) assumes the form

\[ p_y = C \sin (\omega_c t + \varphi_0) \]  

(1.29)
1.4. LANDAU LEVELS

with the integration constants $C$ and $\varphi_0$. The resonance frequency $\omega_c = \frac{Bev_f^2}{E}$ is called the cyclotron frequency. Finally, we derive the motion of $y$ from $p_y$

$$y = -\frac{H}{B^2e^2v_f^2} \frac{dp_y}{dt} + \frac{1}{Be} p_x = -\frac{C}{Be} \cos(\omega_c t + \varphi_0) + \frac{1}{Be} p_x. \quad (1.30)$$

The next step is to solve for the motion of $x$

$$\frac{\partial H}{\partial p_x} = v_f^2 H (p_x - Bey) = C v_f^2 E \cos(\omega_c t + \varphi_0) = \frac{dx}{dt}. \quad (1.31)$$

We can solve the differential equation by integration and find

$$x = x_0 + \frac{C}{Be} \sin(\omega_c t + \varphi_0) \quad (1.32)$$

where $x_0$ is arbitrary. The obtained motion is a circle of radius $r_c = C/Be$ around the position $x = x_0$ and $y = p_x/Be$. Because both coordinates are arbitrary values, the center of the circle can be located anywhere.

We can now solve for the energy $E$ of the system by evaluating the Hamiltonian

$$H = v_f |A| = E. \quad (1.33)$$

The energy of the electron determines the radius $r_c = |A|/Be = E/v_f Be$ and thereby completely fixes the motion. $r_c$ is called the cyclotron radius. It is the most important characteristic of the classical motion.

1.4 Landau levels

We can also consider the problem by the means of quantum mechanics. To obtain the Hamiltonian for electrons in graphene under the influence of a magnetic field we take the Hamiltonian from Eq. (1.22) and again perform the minimal coupling substitution in the Landau gauge as in Eq. (1.25) which yields the Hamiltonian

$$H = v_f (\mathbf{p} + e\mathbf{A}) \mathbf{\sigma} = v_f (p_x - Bey) \sigma_x + v_f p_y \sigma_y. \quad (1.34)$$

The Hamiltonian contains the Pauli matrices $\mathbf{\sigma}$. Because Pauli matrices have the property

$$[A_i, A_j] = 0 \implies (\mathbf{A} \cdot \mathbf{\sigma})^2 = \mathbf{A}^2, \quad (1.35)$$

it is more easy to deal with $H^2$ that is given by

$$H^2 = v_f^2 ((p_x - Bey)^2 + p_y^2)
+ v_f^2 [p_x \sigma_x(p_y \sigma_y - Bex \sigma_y) + (p_y \sigma_y - Bex \sigma_y) p_x \sigma_x]
= v_f^2 ((p_x - Bey)^2 + p_y^2 + \sigma_z \hbar Be). \quad (1.36)$$

By squaring the Hamiltonian states which have the same absolute value of energy become degenerated.
The Hamiltonian commutes with the generator of the translation symmetry in $x$-direction, therefore the solution in the $x$-space can be chosen to be plane waves $\langle x|k_x\rangle = \exp(ik_xx)$. To solve the equation we can decompose the product space $|\psi\rangle = |x\rangle \otimes |y\rangle \otimes |s_z\rangle$ and find the Hamiltonian to be

$$H^2|\psi\rangle = \left[v_f^2(hk_x - Bey)^2 + v_f^2p_y^2 + Behs_z\right]|k_x\rangle \otimes |\psi_y\rangle \otimes |s_z\rangle .$$  \hspace{1cm} (1.37)

The part of the Hamiltonian that operates in the $y$-space has the form of a harmonic oscillator with shifted origin by $\hbar k_x/Be$. We can shift

$$y \rightarrow y' = y - \frac{\hbar k_x}{Be}$$  \hspace{1cm} (1.38)

to bring the problem in the well known harmonic oscillator form

$$H^2 = (v_fBy')^2 + (v_fpy_y)^2 + Behs_z = H_{osc} + Behs_z$$  \hspace{1cm} (1.39)

with an additional energy correction depending on the sublattice degree of freedom. It resembles a harmonic oscillator $H_{osc}$ that only operates in the $y$-space with the mass $m = 1/2v_f^2$ and the resonance frequency $\omega = 2Bev_f^2$.

The eigenvalues of $H_{osc}$ can be obtained by defining the ladder operators

$$a = \sqrt{\frac{Be}{2\hbar}} y' + i\frac{1}{\sqrt{2Be\hbar}} p_y, \quad a^\dagger = \sqrt{\frac{Be}{2\hbar}} y' - i\frac{1}{\sqrt{2Be\hbar}} p_y$$  \hspace{1cm} (1.40)

and identifying $H_{osc} = \hbar \omega(a^\dagger a + 1/2)$. The problem has the known solutions

$$H_{osc} |n\rangle = \varepsilon_n |n\rangle = \hbar \omega(n + \frac{1}{2}) |n\rangle = v_f^2 Be(2n + 1) |n\rangle \quad \text{with } n \in \mathbb{N}_0. \hspace{1cm} (1.41)$$

In the full $H^2$ the eigenstates of $H_{osc}$ are also dependent on $k_x$ because of the shift in $y$, we denote them as $|n, k_x\rangle$. We can now give the full eigenvalue decomposition

$$H^2 |k_x\rangle \otimes |n, k_x\rangle \otimes |s_z\rangle = v_f^2 Be(2n + 1 + s_z) |k_x\rangle \otimes |n, k_x\rangle \otimes |s_z\rangle .$$  \hspace{1cm} (1.42)

Because $s_z = \pm 1$, we can find one state with $E^2 = 0$ and two states for every $E^2 = 2v_f^2 Be n$ with $n$ not equal zero. The energy levels $E = v_f\sqrt{2Be n}$ are called Landau levels. Because we treated the valley degeneracy implicitly, each of these states is again two times degenerated.

We squared the Hamiltonian, so the eigenstates with the same absolute value of energy became degenerate. We want to disentangle the states to get an idea of the sublattice polarization. To do that, we decompose $p_y$ and $y'$ into $a$ and $a^\dagger$ in the Hamiltonian from Eq. (1.34) as suggested by [3]. Then, the problem has the form

$$H = v_f\sqrt{\frac{Be}{2}} \left[-(a^\dagger a)\sigma_z + i(a^\dagger - a)\sigma_y\right].$$  \hspace{1cm} (1.43)

The states that became degenerate for $H^2$ are $|k_x, n, \uparrow\rangle$ and $|k_x, n + 1, \downarrow\rangle$. To find the linear combination that forms the eigenstates to the eigenvalues $E$ and
-E we evaluate $H |k_x, n, s_z\rangle$. We use that the ladder operator satisfy the relations $a |k_x, n, s_z\rangle = \sqrt{n} |k_x, n - 1, s_z\rangle$ and $a^\dagger |k_x, n, s_z\rangle = \sqrt{n + 1} |k_x, n + 1, s_z\rangle$ to find

$$
H |k_x, n, \uparrow\rangle = -v_f \sqrt{2Be\hbar} |k_x, n + 1, \downarrow\rangle, \\
H |k_x, n + 1, \downarrow\rangle = -v_f \sqrt{2Be\hbar(n + 1)} |k_x, n, \uparrow\rangle.
$$

(1.44)

The eigenstates of the problem have again the structure known from the free states

$$
|\psi_+\rangle = \frac{1}{\sqrt{2}} (|k_x, n + 1, \downarrow\rangle + |k_x, n, \uparrow\rangle), \\
|\psi_-\rangle = \frac{1}{\sqrt{2}} (|k_x, n + 1, \downarrow\rangle - |k_x, n, \uparrow\rangle)
$$

(1.45)

in which both sublattices are equally occupied.
Chapter 2

Simulation methods

The aim of this thesis is to understand the properties of transport through a ring shaped graphene device. Because the problem is too complex to be treated analytically, we need some tools to study certain properties.

2.1 Tight-binding simulation

To study the transport properties using quantum mechanics we choose a tight-binding approach. We model the ring in a discrete finite sized lattice as shown in Fig. 2.1 and use the free tight-binding transport simulation package Kwant [5] to do the numerical simulation. Kwant is a free Python package that enables us to study different geometries. It makes use of the matrix inversion library MUMPS [6] that enables efficient solving of the transport problem.

Kwant implements an infinite honeycomb lattice from which we select all the atoms that are inside our geometry. Next, we have to set the onsite potential for every atom and define the hopping amplitude to its neighbors. Finally, we have to parameterize the leads connected to the system. With this information Kwant computes the transport properties of the system. A detailed description of the mathematics that is involved in solving a tight-binding transport problem can be found in [7].

We want to be able to sweep various parameters of the simulation. To do that, we implement a system that takes parameter ranges to be simulated and organizes them into a variable number of groups which can be submitted to batch processing system on a computing cluster. That way we can perform a lot of simulations in parallel without much effort and get the results in reasonable time.

The computing cluster has the disadvantage that the available memory is limited to approximately 2 GB per core. We found that the scaling in memory consumption of the tight-binding simulation is in $O(n^{1.04})$ and the scaling in time consumption is in $O(n^{1.20})$ where $n$ is the number of sites in the simulation as shown in Fig. 2.2. Therefore, we are limited to about $6 \times 10^6$ sites which is approximately $0.015 \mu m^2$ of graphene. The devices that were studied in the experiments [8] have a surface in the order of $1 \mu m^2$ and would overextend the available memory by orders of magnitude.
CHAPTER 2. SIMULATION METHODS

Figure 2.1: The two simulation models we will use. A tight-binding implementation of a ring geometry with the software package Kwant [5] is shown on the left. Note that at this scale the system has only about 1500 sites while the devices that we will study later have $6 \times 10^6$. On the right we show the classical simulation of the ring with ten random trajectories entering the ring from the left side.

Figure 2.2: Plot of the memory and time consumption of the tight-binding simulation dependent on the number of sites in a generic ring geometry. We find that memory consumption scales in $O(n^{1.04})$ and time consumption scales in $O(n^{1.2})$ where $n$ is the number of sites as indicated by the lines. The data of time consumption is scattered because the simulations were done on different computers.
2.2. TRACING OF THE CLASSICAL TRAJECTORIES

To deal with this problem we want to study the properties of the Dirac Hamiltonian

$$H = v_f p \sigma$$

under the scaling transformation

$$x \mapsto \tilde{x} = sx$$

where $s$ is the scaling. As suggested by [7].

Quantum mechanics require that $\tilde{x}$ and $\tilde{p}$ satisfy the canonical commutator relation

$$[\tilde{x}_i, \tilde{p}_j] = [sx_i, \tilde{p}_j] = i\hbar \delta_{i,j}. \quad (2.3)$$

We see that we can choose $\tilde{p} = p/s$. Accordingly, the Hamiltonian of the system transforms as

$$\tilde{H} = v_f \tilde{p} \sigma = \frac{H}{s}. \quad (2.4)$$

It implies that we have to scale up the energy as we scale down the system.

We want to study the system under the influence of a magnetic field. We already discussed this problem in bulk graphene in section 1.4. To perform a correct scaling of the system we require that the energy quantization we found still holds in the scaled system. So we can conclude from

$$\tilde{H}^2 |k_x, n, s_z\rangle = v_f^2 B\hbar (2n + 1 + s_z) |k_x, n, s_z\rangle$$

that the magnetic field should scale according to

$$\tilde{B} = \frac{B}{s^2}. \quad (2.5)$$

To get a good picture of the reality the scaling in the energy and the magnetic field in the simulation have limits. By increasing the energy we get closer to the nonlinear regime of dispersion relation of graphene, that was neglected by linearizing the problem. By increasing the magnetic field we move toward the transport regime known as Hofstadter’s butterfly that shows transport characteristics that are different from the low magnet field regime. To dodge these effects we have to take care that $l_B \gg a$ and $H \ll t$.

2.2 Tracing of the classical trajectories

We want to study the ring in the many mode regime, therefore it is probable that the ring will show some characteristics that can be understood by classical physics. To be able to compare the quantum mechanical simulations with the classical expectations we implement a toolkit in Python to simulate the classical transport of electrons through geometrical defined boundaries such as a ring. The classical description of the problem has the advantage that the dependency of the energy and the magnetic field can be expressed in the single quantity cyclotron radius $r_c$.

We implement the basic set of lines, rays, segments, arcs, and circles to model different geometric boundaries and procedures to calculate intersections.
between the boundary and the trajectory of the electron. We want to study systems that consist of leads through which an electron can enter to a barrier region. In this region it gets scattered and exits the geometry through the same or a different lead. Such as a ring shown in Fig. 2.1. To decide if the trajectory of an electron passes the constriction we trace the trajectory of the electron by repeatedly calculating the next intersection of the path with the boundary of the barrier region and then reflecting it back by using that the angle of reflection is equal to the angle of incidence. Because our initial implementation in Python had a very bad performance, we ported the code to Cython and optimized it until we were able to compute 250 trajectories through a ring per second. Some example trajectories are shown in Fig. 2.1.

To get the transmission we start the trajectory of the electron in a lead that connects to the barrier region. The lead is orientated along the $x$-axis. We start at a fixed $x$-point in the lead. Next, we randomly pick a $y$-position and a direction to start the trace. We check if this choice of initial conditions is propagating in the direction of the barrier. Otherwise we discard it and pick a new position and direction. This is necessary because once we apply a magnetic field a trajectory that initially moves away from the device can be brought into the other direction by the magnetic force. Once we picked a trajectory that propagates, we construct the path through the obstacle to check through which lead it exits.

We will repeat this for many different random initial condition and than compute the transmission $t$ via

$$ t = \frac{T}{n} \quad (2.7) $$

where $T$ is the number of transmitted electrons and $n$ is the number of checked trajectories. The process is a Bernoulli process because the electron either gets reflected or transmitted. Therefore, $T$ will be binomially distributed and we can give the variance to be

$$ \sigma_T^2 = np_T(1-p_T) \quad (2.8) $$

where $p_T$ is the actual transmission probability. The resulting uncertainty in the transmission is given by

$$ \sigma_t = \sqrt{\frac{\sigma_T^2}{n}} = \sqrt{\frac{p_T(1-p_T)}{n}}. \quad (2.9) $$

We will typically calculate $10^5$ trajectories. If we assume a transmission probability $p_T = 0.5$ we will have a uncertainty $\sigma_t \approx 1.5 \cdot 10^{-3}$. 
Chapter 3

Nanoribbons and the connection to the ring

It is important to understand how a straight nanoribbon of graphene behaves because every current in and out of a geometry must be carried through some sort of lead that forms a nanoribbon. Before studying the behavior of a full graphene ring, we therefore want to concentrate on the connection to the ring.

3.1 Zig-zag and armchair

If we perform a tight-binding simulation of a lead we need to define one unit cell of the lead that is repeated over and over to infinity. This repetition must be compatible with the graphene lattice and the direction of the lead must therefore be a linear combination of the lattice vectors of graphene with integer coefficients.

The choice for the smallest unit cell is simply one graphene lattice vector. This type of lead is called zig-zag. Choosing the other lattice vector would result in the exact same geometry because the lattice has a rotational symmetry. The next smallest choice is a linear combination of both lattice vectors \( a_1 + a_2 \). This type of lead is called armchair. Both are shown in Fig. 3.1.

We choose zig-zag leads for our simulations because as shown in [9] the armchair type boundary condition is very special and most generic orientations of nanoribbons in graphene will probably exhibit zig-zag type boundary conditions.

3.2 Dispersion relation of nanoribbons

We start with a zig-zag type lead of the width \( w \) and choose it to point along the \( x \)-axis. We choose it to be symmetric around the \( x \)-axis and refer to upper and lower edge as \( \pm v \). We have to evaluate the eigenvalue equation

\[
H |\psi\rangle = \mathbf{id}_\xi \ v_f \ \mathbf{p} \cdot \mathbf{\sigma} \ |\psi\rangle = E |\psi\rangle
\]

(3.1)
CHAPTER 3. CONNECTION TO THE RING

Figure 3.1: The two most simple forms of leads made of graphene. We show a zig-zag type nanoribbon on the left and an armchair type on the right. The areas marked in green are the unit cells of the lead. We show the translation vector and for the armchair type nanoribbon the decomposition into the graphene lattice vectors. Note that the lattice is rotated in between the two types of nanoribbons.

that describes the motion of electrons in graphene under the termination condition

\[
\langle \pm v, y, \xi, s_z | \tau_z \otimes \sigma_z | \psi \rangle = \pm \langle \pm v, y, \xi, s_z | \tau_z \otimes \sigma_z | \psi \rangle
\]

(3.2)
derived in [9] where \(\tau_i\) denote the Pauli matrices on the valley space.

To study the eigenenergies of this Hamiltonian we can square it to get rid of the Pauli matrices. We obtain

\[
H^2 = v_f^2 (p_x^2 + p_y^2).
\]

(3.3)
We see that this Hamiltonian together with the boundary condition is translational invariant in the \(x\)-direction. Therefore, we can reduce the problem to one dimension by using the wave solution

\[
\langle x | k_x \rangle = e^{ik_xx}, \quad H^2 | \psi \rangle = \text{id}_x \otimes H^2_y | k_x \rangle \otimes | \psi_y \rangle, \quad H^2_y = v_f^2 (\hbar^2 k_x^2 + p_y^2)
\]

(3.4)
in the \(x\)-space. The eigenvalue problem can now be formulated as the differential equation

\[
E^2 \langle y, \xi, s_z | \psi_y \rangle = v_f^2 (\hbar^2 k_x^2 - \hbar^2 \partial_y^2) \langle y, \xi, s_z | \psi_y \rangle
\]

(3.5)
in the \(y\)-space. We can rewrite the problem as

\[
-(k_f^2 - k_x^2) \langle y, \xi, s_z | \psi_y \rangle = \partial_y^2 \langle y, \xi, s_z | \psi_y \rangle
\]

(3.6)
where \(k_f = E/v_f \hbar\) is the Fermi wavevector. We want to use \(k_y^2\) as a short notation for \(k_f^2 - k_x^2\).

The solution of the problem is derived in [3]. They find that the termination conditions allow both real and imaginary solutions for \(k_y\). The imaginary solutions are relevant for edge states that are of importance in the few mode regime as we are interested in the many mode regime only the quantization for real \(k_y\)

\[
k_x = \frac{k_y}{\tan(wk_y)}
\]

(3.7)
3.3. THE INFLUENCE OF A MAGNETIC FIELD

Figure 3.2: The analytic calculation (lines) and the tight-binding simulation (dots) of the dispersion relation of a zig-zag type nanoribbon with width $w = 400a$ around the $K$ point is shown. The offset in the momentum is given by the location of the Dirac point at $2\pi/3a$. The part of the simulation that is not covered by the analytic calculation are edge states. We only show states with positive energy.

is of interest to us. The conductivity of nanoribbon at a certain energy $E$ is quantized and given by the number of modes that propagate times the conductance quantum $G_0 = 2e^2/h$. The quantization condition in Eq (3.7) implies that a new mode is added to the dispersion relation whenever $\tan(\frac{wk_f}{2})$ is divergent. We can conclude that a change in the conductivity will occur whenever $wk_f = (n + 1/2)\pi$.

We performed a tight-binding simulation of a graphene nanoribbon with zig-zag type boundary conditions and compare the results with the analytically found solution as shown in Fig. 3.2.

3.3 The influence of a magnetic field

Now we want to study the behavior of an ideal lead under the influence of a magnetic field. The free solution with no boundary conditions in bulk graphene was done in section 1.4. Since we did not brake the translational symmetry that was used in the derivation of the Hamiltonian in Eq. (1.36), we can solve it with respect to the confining hard wall. Because we want to apply a semi-classical solution, we bring the problem into the position space representation

$$ \langle y, k_x, s_z | \psi \rangle = \psi_{s_z, k_x}(y), $$

$$ v_f^2 ((\hbar k_x + B ey)^2 - \hbar^2 \partial_y^2 + Beh s_z) \psi_{s_z, k_x}(y) = E^2 \psi_{s_z, k_x}(y). $$

(3.8)
CHAPTER 3. CONNECTION TO THE RING

We rearrange the equation in a way that the differentiation stands without prefactor. In the form
\[
\left((k_x + \frac{Be}{\hbar} y)^2 + \frac{Be}{\hbar} s_z - \partial_y^2\right)\psi_{s_z,k_x}(y) = \frac{E^2}{v^2 f^2} \psi_{s_z,k_x}(y) \tag{3.9}
\]
we can identify a new important length scale in the description of the problem. It is given by \(\frac{Be}{\hbar} = l_B^{-2}\) where \(l_B\) is the magnetic length. The magnetic length is defined to be the radius of a circle through which one magnetic flux quantum \(\phi_0 = e/h\) flows. Additionally, we can identify the Fermi wave vector \(k_f\) and conclude
\[
\left((k_x + \frac{y}{l_B^2})^2 + \frac{s_z}{l_B^2} - \partial_y^2\right)\psi_{s_z,k_x}(y) = k_f^2 \psi_{s_z,k_x}(y). \tag{3.10}
\]
This differential equation has a form that can be approximated using the semi-classical approach
\[
\int_a^b \sqrt{(k_x + \frac{y}{l_B^2})^2 - k_f^2 + \frac{1}{l_B^2}} \, dy' = \pi (n + \gamma) \quad \text{with} \quad n \in \mathbb{N}_0 \tag{3.11}
\]
where \(\gamma\) is the Maslov index of the problem. We can simplify the integration by the substitutions
\[
y' = y + k_x l_B^2, \quad \varepsilon_\pm = k_f^2 \pm \frac{1}{l_B^2} \tag{3.12}
\]
so that we obtain
\[
\frac{1}{l_B^2} \int_a^b \sqrt{y'^2 - \varepsilon_\pm l_B^2} \, dy' = \left. \frac{l_B^2 \varepsilon_\pm}{2} \sin^{-1}\left(\frac{y'}{l_B^2 \sqrt{\varepsilon_\pm}}\right) + \frac{y'}{2} \sqrt{\varepsilon_\pm - y'^2 l_B^2}\right|_a^b. \tag{3.13}
\]
The integration has a nice geometric interpretation: it measures the area of the overlap from the lead and the circle that a free electron in bulk material would describe [10]. The interpretation is shown in Fig. 3.3. By multiplying with \(l_B^{-2}\) it gives \(\pi\) times the number of magnetic flux quanta that flows through this area. We can find the cyclotron radius \(r_c\) from the classical discussion of electrons in graphene under the influence of a magnetic field in \(\sqrt{\varepsilon_\pm} l_B^2\), but with an additional correction due to the setting of the pseudo spin \(s_z\), that was not part of the classical discussion.

To evaluate the definite integration we have to fix the integration limits \(a\) and \(b\). At this point, we have to make a case distinction and decide whether the classic return point is given by the hard wall or the magnetic field. We find the limits to be
\[
a = \min \left(\sqrt{\varepsilon_\pm} l_B^2, v - k_x l_B^2\right) = \begin{cases} \sqrt{\varepsilon_\pm} l_B^2, & \text{if } \sqrt{\varepsilon_\pm} < \frac{v}{l_B^2} - k_x, \\ v - k_x l_B^2, & \text{otherwise}, \end{cases}
\]
\[
b = \max \left(-\sqrt{\varepsilon_\pm} l_B^2, -v - k_x l_B^2\right) = \begin{cases} -\sqrt{\varepsilon_\pm} l_B^2, & \text{if } \sqrt{\varepsilon_\pm} < \frac{v}{l_B^2} + k_x, \\ -v - k_x l_B^2, & \text{otherwise}. \end{cases}
\tag{3.14}
\]
3.3. THE INFLUENCE OF A MAGNETIC FIELD

We can identify three different types of states two types are shown in Fig. 3.3. First, there are states that are limited on both sides by the hard wall. These are magnetically perturbed states equivalent to those in a lead without magnetic field. Then, there are states that are limited on one side by the hard wall and on the other side by the magnetic field. These states are called skipping orbit states. They make a cyclic motion, but before performing a complete turn, they hit the wall and get scattered back. Finally, there are states that are completely confined by the magnetic field. They have no classical interaction with the wall and are equivalent to the states in the quantum mechanical discussion of electrons in bulk graphene.

States of the first kind only appear if

\[ \sqrt{\varepsilon_{\pm}} \geq \frac{v}{l_B} + k_x \land \sqrt{\varepsilon_{\pm}} \geq \frac{v}{l_B} - k_x \implies l_B^2 \sqrt{\varepsilon_{\pm}} \geq v. \]  

(3.15)

The quantity \( l_B^2 \sqrt{\varepsilon_{\pm}} \) has appeared in the integration as the equivalence of the cyclotron radius \( r_c \). If we neglect the influence of the lattice pseudo spin we can give the approximate condition

\[ 2r_c \geq w \]  

(3.16)

for the existence of states that touch both sides. The regime where the cyclotron
Figure 3.4: A plot of the simulated conductivity of a zig-zag type nanoribbon of width $w = 40$ nm in the influence of a magnetic field $B$ at the energy $E$ (A) and the conductivity for the fixed energy $E = 0.36t$ (B). Additionally, we show the approximation found in Eq. (3.17).

diameter $2r_c$ is smaller than the width of the constriction is called quantum Hall regime. In that transport regime the complete transport takes place in channels that reach only $2r_c$ deep into the material.

To apply the quantization rule in Eq. (3.11), we would need to determine the Maslov index $\gamma$. Finding the Maslov index is not trivial when the wavefunction is confined by the smooth magnetic field but the hard wall is still present in the classical forbidden region. In that case the Maslov index evolves steady from $1/2$ to $1/4$ when the wall is at infinite distance as shown together with an appropriate approximation in [10]. An additional problem for zig-zag nanoribbons in graphene is that the termination condition does not have the simple form $\psi(\pm v) = 0$ as assumed for the derivation in [10].

To get an approximation for the conductance of an nanoribbon under the influence of the magnetic field we can solve for $n(E, k_x)$ in the quantization condition in Eq. (3.11) and use it as an approximation for the number of modes with momentum $k_x$ and a energy smaller than $E$. Then, we can use

$$G = 2G_0 n(E, k_x = 0)$$

as an approximation for the conductivity. The additional factor of 2 is to treat the two valley configurations. We will neglect the influence of the Maslov index and the corrections due to the pseudo spin. A comparison between the approximation and a tight binding simulation is presented in Fig. 3.4

### 3.4 Impedance matching

To study the electric properties of a device in an experiment one needs to connect it to measurement equipment. Therefore, wires that connect to the
3.4. IMPEDANCE MATCHING

Figure 3.5: The transmission through the impedance matching test setup and the maximal possible conductivity of the undoped lead is shown in A and the corresponding reflection for modes that enter from the undoped side is shown in B. We show a sketch of the impedance matching test setup in C. It is parameterized by the length of the matching region $l_{\text{match}}$ and the indicated rotation of the region.

device are necessary. These leads need to be much wider than the system to not dominate the behavior of the experiment. Connecting wide leads in a simulation would be numerically very demanding since the computational effort is dependent on the number of lattice sites. To be able to simulate many modes that connect down to the area of interest we dope the wires to a high onsite potential of $E_{\text{dope}} = 1.1t$. The leads do not show graphene characteristics at this doping and model the metallic connections used in experiments.

A problem that arises when connecting a highly doped lead to the usual graphene is that an impedance mismatch occurs at the transition that leads to an almost complete reflection of the entering modes. To be able to transport the incoming modes into the undoped area we need to introduce an impedance matching region in which the onsite potential is steadily decreased to allow certain modes from the highly doped region to couple to modes in the device.

In [7] the two models of linear and reciprocal reduction of the onsite energy in different orientations were studied as impedance matching regions. They concentrated on the impedance matching in the low energy regime up to 13 modes in the undoped lead. We want to study transport at up to 45 modes in the undoped lead, therefore we implement the test setup for the impedance matching shown in Fig. 3.5. We find that in our regime for a zig-zag type nanoribbon a reciprocal reduction of the onsite potential that is rotated by 0.43 rad shows optimal transmission to the undoped lead. For leads of width $w = 40\,\text{nm}$ we will use a length of the impedance matching region $l_{\text{match}} = 20\,\text{nm}$.

Care must be taken when studying the quantum Hall regime because we
found that in the doped area modes that would normally be protected by the strong magnetic fields and the small cyclotron radius can interact with each other. For this reason, we must not use the impedance matching when studying effects that are related to quantum Hall channels.

3.5 T-Junction

To get an insight in the way the electrons enter the ring we first study the transport through a T-junction. We model the geometry of a T-junction with tight-binding methods and perform a transport simulation dependent on the applied magnetic field. Because it is not trivial to implement connections to a system that point in different directions, we also implement half of the ring. A sketch of the setup is shown in Fig. 3.6. We also implemented a classical transport simulation for a T-junction. Both results can be found in Fig. 3.6.

We can now compare the classical transmission with the quantum mechanical transmission. We find that in both cases the applied magnetic field breaks the symmetry of the two arms a and b and creates one arm through which the transport happens favorably. The major difference between the quantum mechanical and the classical description is the fact that in the classical simulation there is no backscattering when entering the T-junction through the arm a or b.
Figure 3.6: The simulated transport through a T-junction is shown. The model shown in A is used for the classical simulation. The model in B is used for studying the transport properties with tight-binding methods. We added a highly doped lead and an impedance matching region at the entrance o. Therefore, we cannot give the quantum mechanical reflection for o. In C we present the simulation results. We normalized the quantum mechanical observed conductivity using the approximation in Eq. (3.17).
Chapter 4

Transport through a graphene ring

Finally, we want to study a ring made of graphene. First, we want to define the way we talk about the geometry. The ring is parameterized by the inner radius \( r_i \), the outer radius \( r_o \), the width \( w \) of the leads that connect to the ring, and the width of the arm of the ring \( w_r \). We want to orientate our coordinate system such that the connecting lead points along the \( x \)-axis and orientate the graphene lattice in the tight-binding such that the leads that connect to the system are of zig-zag type. The setup is shown in Fig. 4.1.

4.1 Experimental data and the parameter for the simulation

The aim of this thesis is to theoretically understand certain properties that were observed by \[8\]. They have achieved to fabricate graphene rings in very high quality using graphene that is encapsulated between two sheets of hexagonal boron nitride. These sandwiches are known to have high electron mobilities and therefore will exhibit properties close to pure graphene. The geometry that was studied has an inner radius \( r_i = 400 \text{ nm} \), an outer radius \( r_o = 800 \text{ nm} \), and a width \( w = 400 \text{ nm} \). Its electrical properties were measured at temperatures as low as 36 mK and in magnetic fields up to 8 T.

To perform our simulations we need to determine the Fermi energy \( \varepsilon_f \) of the system because that will give us the energy \( E \) with respect to the Dirac cone at which we perform the simulation. In the experiment the parameter that controls the Fermi energy is the backgate voltage \( V_{BG} \). A voltage that is applied at the back of the device and affects the charge carrier density \( n \). At a backgate voltage of \(-15 \text{ V}\) a charge carrier density of \( 7.6 \times 10^{11} \text{ cm}^{-2} \) was found \[8\].

The charge carrier density \( n \) is given by the integration about the density of states to the Fermi energy

\[
n = 2 \int \int \frac{d^2k}{(2\pi)^2} \theta[E(k) - \varepsilon_f]
\]

(4.1)
Figure 4.1: A diagram of a ring. We show the orientation of the axis $x$ and $y$. The parameters that characterize the geometry of the ring are: The width $w$ of the connected leads, the radius of the inner hole $r_i$, the outer radius of the ring $r_o$, and the width of the arm $w_r$. The graphene lattice is orientated such that the leads are of zig-zag type.

where $\theta$ is the Heaviside step function and the factor of 2 is to respect the two spin configurations of the electrons. Because of the linear energy-momentum relation, we can evaluate the integration to be

$$n = 2 \cdot \int \left| k \right| < k_f \frac{d^2k}{(2\pi)^2} = 2 \cdot \frac{k_f^2}{2\pi} = \frac{\varepsilon_f^2}{\pi v_f^2 \hbar^2}. \quad (4.2)$$

The additional factor of 2 is necessary to treat the two valley configurations of graphene. We can solve for $\varepsilon_f = \sqrt{n\pi v_f \hbar}$ and find $\varepsilon_f \approx 0.035t$.

The ring in the experiment has a surface of $\pi r_o^2 - \pi r_i^2 \approx 1.5 \mu m^2$ and consist of about $6 \times 10^8$ carbon atoms which is about 100 times more than we are able to simulate. We therefore have to scale down the geometry by a factor $s = 0.1$ to meet the constraints of the simulation. It implies that we have to scale up the energy to $\varepsilon'_f = 10 \varepsilon_f \approx 0.35t$ and scale up the magnetic field to $B' = 100B$. In the following, we will use the scaled values that are present in our simulation.

Wide leads with a metalization are used in the experiment to connect the ring to the measurement equipment. To model the wide lead and the metal contact we use high doped leads together with the impedance matching method described in section 3.4. We add the impedance matching in the distance $l_s = 20$ nm from the entrance to the ring. That is approximately the same distance in which the second contact for a four terminal measurement is placed in the experiments.

We tried to reproduce the magneto-conductance trace that was observed in the experiments with this setup. In the following sections, we want to discuss
4.2. INCREASE OF CONDUCTIVITY

We observe a characteristic increase of the conductivity when applying a magnetic field followed by a characteristic decrease. This observation is consistent with the experimental results as shown in Fig. 4.2.

The increase in the conductivity can be understood in a classical picture of the problem. Once we turn on the magnetic field, the electrons that enter the ring are subject to a magnetic force. This force breaks the symmetry between the two arms of the ring and one arm becomes favorable for the entering electrons. We already observed this behavior in simulations of the T-junction. Due to this effect, the reflection back into the lead gets reduced. In addition, the magnetic force pushes the electrons in the magnetically favorable arm in the outer direction and makes it more probable for them to exit through the other lead without performing a full cycle in the ring.

The effect evolves steady until the magnetic field is strong enough to force the electrons into quantum Hall channels. In section 3.3, we found in a semi-
Figure 4.3: The simulated transmission through a ring with width \( w = w_r = 40\,\text{nm} \) is shown. The remnants of the conductance quantization in the width \( w_r \) are clearly visible. Compare Fig. 3.4.

classical picture the condition

\[ 2r_e = w \quad (4.3) \]

for the transition to the quantum Hall regime. That is consistent with the maximum we found in the simulated magneto-conductance trace.

The following decrease of conductivity at high magnetic fields can be understood by the transport properties of the quantum Hall regime, characterized by the impossibility for the classical trajectory of an electron to reach both boundaries of the constriction. In that regime, the quantum Hall channel along the edge is completely formed and the geometry of the ring has no effect on the transmission. The conductivity is then independent of the geometry.

### 4.3 Conductance quantization

We observe steps in the simulated conductance dependent on the applied magnetic field. We want to compare these steps with the features that are present in the experimental data. Both are indicated in Fig. 4.2. To determine the nature of the step in the simulation we compute the magneto-conductance trace at different energies. The results are shown in Fig. 4.3. We find that the effect that forms the step in our initial simulation creates lines of minima in the conductance dependent on the energy and the applied magnetic field. We compare the structure of the feature with the conductance of a zig-zag nanoribbon under the influence of a magnetic field discussed in section 3.3 and find that the feature appears with the same periodicity as the conductance quantization in the width of the lead \( w \) or the width of the arms \( w_r \) as both parameters are equal in our simulation. We conclude that the features are remnants of the quantized conductivity in channels of the width \( w \) or \( w_r \).
Figure 4.4: A plot of the simulated conductivity of graphene rings with reduced armwidth \( w_r \) in comparison to the simulation presented in Fig 4.3. We show the conductance for a ring with \( w_r = 30 \text{ nm} \) (A) and for a ring with \( w_r = 20 \text{ nm} \) (B). We indicate the expected energy levels for the quantization at vanishing magnetic fields.

To demonstrate that the quantization is not an remnant of the wires that connect to the ring, we perform simulations with decreased arm width \( w_r \) and find that in that case the feature behaves as the conductance quantization for a ziz-zag lead of the now smaller width \( w_r \) as shown in Fig. 4.4. Additionally, we find that the maximum of conductivity gets shifted to higher magnetic fields as now the cyclotron radius needs to be smaller than half of the reduced \( w_r \) to bring the complete system into the quantum Hall regime.

Conductance quantization is an effect on the scale \( w_r k_f \) with additional modifications through the magnetic field as discussed in section 3.3. Therefore, the effect can also be observed for vanishing magnetic fields in the dependence of the conductance on the energy.

The signature that is present in the experimental data can not be a consequence of conductance quantization because the feature in the experiment is not present at \( B = 0 \) and has not the characteristic dependency on the energy that is visible in Fig. 4.3.

### 4.4 Signatures of ballistic transport

We want to reproduce the dominant features of the experimental data in our simulation. We found that the presence of conductance quantization dominates the structure in the magneto-conductance trace. To uncover other present structures we decide to break the fixed mode number in the arms of the ring by introducing edge roughness. The actual structure of edge roughness in an experiment is not known and could only be approximated because our simulation is scaled down by factor 10. Therefore, we apply a very simple form
Figure 4.5: A plot of the conductance of the ring with edge roughness as described in section 4.4. In A we show how the step evolves when increasing the parameter $a$ that parameterizes the intensity of the roughness. $a = 0$ nm represents an undistorted ring. We pick a slightly different energy $E = 0.036t$ in comparison to 4.2 that even without edge roughness shows less remnants of conductance quantization. In B, we show the conductance dependent on the energy $E$ and the magnetic field. We find that the step behaves like a cyclotron radius and give an indication of the cyclotron radius that corresponds to the end of the step as a line in B.

of edge disorder without the intention to create an exact representation of the actual experiment. We modulate the outer radius of the graphene ring $r_0$ with a sinusoidal. This model has two parameters, the amplitude of the modulation $a$ and the number of repetitions along the circumference $n$.

As initial values we choose $n = 20$ and $a \leq 6$ nm. With these modifications in our model we see a step evolve in the magneto-conductance trace as shown in Fig. 4.5. If we mark the minimum that is present at the end of the step in the plot that shows the conductance dependent on the magnetic field and the energy we find that the minimum can be parameterized as a constant cyclotron radius $r_c \approx 25$ nm. It is shown in Fig. 4.5. In the experiment the feature also behaves like a cyclotron radius.

The conductance in a tight-binding simulation is given by the sum above the transmission probabilities of the entering modes times the conductance quantum $G_0$. We hope to get an insight in the source of the step by analyzing the conductance resolved by the momenta of the entering modes. This is difficult with the high doping in the leads because we lose a lot of information about the mode that actually enters the ring. Therefore, we remove the doping and the impedance matching region that were used to model the contacts to the system and compute the transmission through the ring resolved by the entering mode for both the distorted and the undistorted system. We show the result of the simulation in Fig. 4.6.
4.4. SIGNATURES OF BALLISTIC TRANSPORT

Figure 4.6: A plot of the transmission probability through the ring sorted by the momentum of the entering mode for a system with smooth edge (A) and for a system with edge roughness (B). The leads to the system are of zig-zag type, we only show one of the Dirac cones. We indicate the boundary between edge modes and normal modes. All modes above the line are edge modes. The marked minimum of the transmission probability around $B = 0.4 \, \text{T}$ in the system with edge roughness is the source of the step feature in Fig. 4.5.

The structure that is responsible for the step in the distorted system is visible as minima of transmission probabilities for many modes at once. We also find similar structures in the transmission probabilities for the undistorted system. In the following, we will only concentrate on the features in the undistorted ring because they give insight in the transport properties, but are not dominated by conductance quantization.

To understand the drop of the transmission probability we pick a fixed mode and calculate the wave function for different magnetic fields. These are shown in Fig. 4.7. The wave function shows a clear defined path that almost resembles a classic trajectory that performs skipping orbits along the outer boundary. Because the wave function interacts mainly with the outer boundary, we expect a significant dependency of the effect based on the outer radius $r_o$. To demonstrate that we perform a tight-binding simulation with variable outer radius $r_o$ at a fixed arm width $w_r = w$. We pick the mode with the fourth highest momentum into ring, because for that mode the minima structure is distinct, and plot the transmission of this mode dependent on the magnetic field and the outer radius of the ring $r_o$. This is shown in Fig. 4.8. We observe that the magnetic field at which transmission minima occur depends significantly on the outer radius $r_o$.

Both the fact that the wave function resembles a trajectory and that the feature is created by a many mode effect suggests that it is a classical phenomenon. To be able to compare the tight-binding simulation with the classical physics we also implement the ring in the classical simulation model described in sec-

\[
\begin{align*}
\text{Fig. 4.6: A plot of the transmission probability through the ring sorted by the momentum of the entering mode for a system with smooth edge (A) and for a system with edge roughness (B). The leads to the system are of zig-zag type, we only show one of the Dirac cones. We indicate the boundary between edge modes and normal modes. All modes above the line are edge modes. The marked minimum of the transmission probability around } B = 0.4 \, \text{T in the system with edge roughness is the source of the step feature in Fig. 4.5.}
\end{align*}
\]
Figure 4.7: The tight-binding transport through a ring at a fixed energy $E = 0.036t$ is shown. We plot only one entering mode for four different magnetic fields. We see how the transmission maximum $n = 5$ in A changes under an increasing magnetic field through two configurations with lower transmission in B and C until the next higher transmission maximum $n = 6$ is present in D.
Figure 4.8: A plot of the transmission of the lead mode with the fourth highest momentum in the $x$-direction dependent on the outer diameter of the ring $d_o = 2r_o$ is shown in A. We keep the width of the ring fixed at $w = 40 \text{ nm}$. In B we show the classic transmission through the ring, dependent on the inner ring diameter and the ratio between the cyclotron radius $r_c$ and the width $w$. We add a model for the visible structure given by $\pi/2 \arctan(r_c/r_o) = n$ as derived in section 4.4. The dark blue artifacts in A are due to crashed simulations.

...
Figure 4.9: A sketch of the repetition condition described in section 4.4 for the orders \( n = 3 \) to \( n = 6 \) is shown.

Figure 4.10: Graph of the measured conductance of a graphene ring with \( w = 400 \text{ nm}, r_i = 400 \text{ nm}, \) and \( r_o = 800 \text{ nm} \) at a backgate voltage \(-15 \text{ V}\) by [8] in arbitrary units. We also show the classical transmission probability simulated for that device. The location of the first minimum in the simulation at \( B \approx 0.37 \text{ T} \) fits reasonable to the location of the step feature in the experimental data.
4.5 AHARONOV-BOHM OSCILLATIONS

Aharonov-Bohm oscillations are a quantum interference effect that can be understood by modeling the ring as a double slit experiment in which an electron picks the upper and the lower arm of the ring and interferes at the exit. The electron picks up the phase shift $\varphi$ while moving along the path $\gamma$ in the influence of the vector potential $A$ associated to the magnetic field $B$. $\varphi$ is given by

$$\varphi = \frac{e}{\hbar} \int_{\gamma} A \cdot dx.$$  \hspace{1cm} (4.5)
Figure 4.12: In A the oscillations with the highest frequencies that can be found in the simulated magneto-conductance trace are shown. In B we show the Fourier transformation of the magneto-conductance trace for the ring with inner radius $r_i = 40\,\text{nm}$ and outer radius $r_o = 80\,\text{nm}$. We mark the magnetic frequencies that correspond to $A_i = \pi r_i^2$ and $A_o = \pi r_o^2$. The same was done in C for a ring with increased inner radius $r_i = 60\,\text{nm}$. For the ring with reduced width the next higher order of Aharonov-Bohm oscillations is visible in the Fourier spectrum.
4.5. AHARONOV-BOHM OSCILLATIONS

To study the interference only the phase difference between the path along the upper arm of the ring $\gamma$ and the path along the lower arm of the ring $\gamma'$ is of interest. Calculating the phase difference $\Delta \varphi$ along these two paths is equivalent to evaluate the phase picked up when the electron moves along the closed path $C$ that consist of $\gamma$ followed by $\gamma'$ in reverse. Because we study the constant magnetic field $B$, the integration can be solved by Stokes’s theorem to be

$$\Delta \varphi = \frac{e}{\hbar} A_C B$$

(4.6)

where $A_C$ is the area enclosed by $C$. The area is unique because the problem is two dimensional. That leads to a magnetic frequency $f_B = e/2\pi \hbar A_C$ associated to the area $A_C$. More on the topic of Aharonov-Bohm oscillations can be found in [8].

We find oscillations in the simulation that have high frequencies in comparison to the other effects discussed before. They are visible for all energies we simulated. But they do not have a well defined sinusoidal shape. This is also visible in the Fourier spectrum of the conductance trace. The oscillations and the Fourier transformation are shown in Fig. 4.12. We can compute the frequencies that are associated with the area of the inner barrier of the ring to be $121 \text{ T}^{-1}$ and for the area enclosed by the outer radius of the ring to be $486 \text{ T}^{-1}$. When we mark these frequencies in the Fourier spectrum, we can find that between those frequencies lies a diffuse maximum. Therefore, the oscillations are indeed Aharonov-Bohm oscillations.

We do not obtain a pure oscillation because there is no prominent enclosed area for the different paths of the electrons. This results in a diffuse wide maximum in the Fourier spectrum. To be able to observer higher quality oscillations we have to define a clearer path for the electrons that can be done by decreasing the width $w_r$ of the ring. Then the inner barrier becomes more prominent as an area that is enclosed by electron trajectories. To prove it we also perform simulations with an increased inner radius $r_i = 60 \text{ nm}$ that implies a reduced arm width of $w_r = 20 \text{ nm}$. We are able to observe better defined Aharonov-Bohm oscillations which is also visible in the Fourier spectrum. We now find a peak between the old frequency associated with the outer ring and the new frequency $273 \text{ T}^{-1}$ that results from the changed inner radius. Now we can also identify contributions of Aharonov-Bohm oscillations in higher order. These are contribution by path that lead around the inner barrier multiple times.
Chapter 5

Summary

In this thesis, we first gave an introduction to the electronic properties of bulk graphene. Next, we introduced two simulation methods that can be used to study certain transport properties. Because we want to understand the transport through a ring, we first analyzed the way electrons enter a ring geometry by studying the behavior of nanoribbons and T-junctions. Finally, we studied the transport through a complete graphene ring.

We were able to reproduce certain aspects of the data measured by [8]. At the beginning of our investigation we gave an insight into the rise followed by a decrease of the conductivity at rising magnetic fields. Then, we studied the effect of conductance quantization. We argued that this type of modulation is not present in the experimental data and tried to uncover more of the structure by introducing edge roughness to our model. We found an effect of classical transport associated to the geometry of the ring that leads to oscillations in the magneto-conductance trace. We presented a model for the behavior of this effect and were able to reproduce it in a tight-binding simulation. In the end, we studied Aharonov-Bohm oscillations and showed that the purity of the observed oscillations are related to the width of the ring.
Bibliography


