Linköping Studies in Science and Technology
Dissertations No. 1837

**Quantum scattering and interaction
in graphene structures**

Anna Orlof

Department of Mathematics, Division of Mathematics and Applied Mathematics
Linköping University, SE-581 83 Linköping, Sweden
Linköping 2017

Linköping Studies in Science and Technology. Dissertations No. 1837

Quantum scattering and interaction in graphene structures

Copyright © Anna Orlof, 2017

Division of Mathematics and Applied Mathematics

Department of Mathematics

Linköping University

SE-581 83, Linköping, Sweden

anna.orlof@liu.se

ISSN 0345-7524

ISBN 978-91-7685-562-1

Printed by LiU-Tryck, Linköping, Sweden 2017

Abstract

Since its isolation in 2004, that resulted in the Nobel Prize award in 2010, graphene has been the object of an intense interest, due to its novel physics and possible applications in electronic devices. Graphene has many properties that differ it from usual semiconductors, for example its low-energy electrons behave like massless particles. To exploit the full potential of this material, one first needs to investigate its fundamental properties that depend on shape, number of layers, defects and interaction. The goal of this thesis is to perform such an investigation.

In paper I, we study electronic transport in monolayer and bilayer graphene nanoribbons with single and many short-range defects, focusing on the role of the edge termination (zigzag vs armchair). Within the discrete tight-binding model, we perform analytical analysis of the scattering on a single defect and combine it with the numerical calculations based on the recursive Green's function technique for many defects. We find that conductivity of zigzag nanoribbons is practically insensitive to defects situated close to the edges. In contrast, armchair nanoribbons are strongly affected by such defects, even in small concentration. When the concentration of the defects increases, the difference between different edge terminations disappears. This behaviour is related to the effective boundary condition at the edges, which respectively does not and does couple valleys for zigzag and armchair ribbons. We also study the Fano resonances.

In the second paper we consider electron-electron interaction in graphene quantum dots defined by external electrostatic potential and a high magnetic field. The interaction is introduced on the semi-classical level within the Thomas Fermi approximation and results in compressible strips, visible in the potential profile. We numerically solve the Dirac equation for our quantum dot and demonstrate that compressible strips lead to the appearance of plateaus in the electron energies as a function of the magnetic field. This analysis is complemented by the last paper (VI) covering a general error estimation of eigenvalues for unbounded linear operators, which can be used for the energy spectrum of the quantum dot considered in paper II. We show that an error estimate for the approximate eigenvalues can be obtained by evaluating the residual for an approximate eigenpair. The interpolation scheme is selected in such a way that the residual can be evaluated analytically.

In the papers III, IV and V, we focus on the scattering on ultra-low long-range potentials in graphene nanoribbons. Within the continuous Dirac model, we perform analytical analysis and show that, considering scattering of not only the propagating modes but also a few extended modes, we can predict the appearance of the trapped mode with an energy eigenvalue slightly less than a threshold in the continuous spectrum. We prove that trapped modes do not appear for energies slightly bigger than a threshold or far from it, provided the potential is sufficiently small. The approach to the problem is different for zigzag vs armchair nanoribbons as the related systems are non-elliptic and elliptic respectively; however the resulting condition for the existence of the trapped mode is analogous in both cases.

Populärvetenskaplig sammanfattning

Sedan isoleringen av grafen 2004, vilket belönades med Nobelpriset 2010, har intresset för grafen varit väldigt stort på grund av dess nya fysikaliska egenskaper med möjliga tillämpningar i elektronisk apparatur. Grafen har många egenskaper som skiljer sig från vanliga halvledare, exempelvis dess lågenergi-elektroner som beter sig som masslösa partiklar. För att kunna utnyttja dess fulla potential måste vi först undersöka vissa grundläggande egenskaper vilka beror på dess form, antal lager, defekter och interaktion. Målet med denna avhandling är att genomföra sådana undersökningar.

I den första artikeln studerar vi elektrontransporter i monolager- och multilagergrafennanoband med en eller flera kortdistanseveningar, och fokuserar på inverkan av randstrukturen (zigzag vs armchair), härfter kallade zigzag-nanoband respektive armchair-nanoband. Vi upptäcker att ledningsförmågan hos zigzag-nanoband är praktiskt taget okänslig för defekter som ligger nära kanten, i skarp kontrast till armchair-nanoband som påverkas starkt av sådana defekter även i små koncentrationer. När defektkoncentrationen ökar så försvinner skillnaden mellan de två randstrukturerna. Vi studerar också Fanoresonanser.

I den andra artikeln betraktar vi elektron-elektron interaktion i grafen-quantprickar som definieras genom en extern elektrostatisk potential med ett starkt magnetfält. Interaktionen visar sig i kompressibla band (compressible strips) i potentialfunktionens profil. Vi visar att kompressibla band manifesteras i uppkomsten av plattåer i elektronenergierna som en funktion av det magnetiska fältet. Denna analys kompletteras i den sista artikeln (VI), vilken presenterar en allmän feluppskattning för egenvärden till linjära operatorer, och kan användas för energispektrum av quantprickar betraktade i artikel II.

I artiklarna III, IV och V fokuserar vi på spridning på ultra-låg längdistanspotential i grafennanoband. Vi utför en teoretisk analys av spridningsproblemet och betraktar de framåtskridande vågor, och dessutom några utökade vågor. Vi visar att analysen låter oss förutsäga förekomsten av fångade tillstånd inom ett specifikt energiomtervall förutsatt att potentialen är tillräckligt liten.

Acknowledgements

Above all, I would like to express gratitude to my supervisors Vladimir Kozlov and Igor Zozoulenko. Thank you for your continuous guidance and support. Vladimir, thank you for your patience and for keeping your doors open whenever I needed. Igor, thank you for all your advices and for pushing me to do constructive stuff.

I am grateful to my collaborators. To Artsem Shylau, for great discussions about physics, work and after work time in Denmark and for introducing me to POV-Ray. To Fredrik Bentsson for all the help, discussions and above all the dynamical work environment that I liked so much. To Sergey Nazarov and Julius Ruseckas, for answering all my questions.

I am thankful to my work-mate Arpan, for discussions about research and all interesting deviations from it.

The work on this thesis was a piece of my life. That is why I would like to mention all my current/former PhD friends that made it a great experience: Alexandra – for talks about babies, to Leslie for tequila time, to Mikael for trying to teach me overhead service, to David for discussions about mathematics and the zoo, to Viktor for letting me and my little family stay in his flat when we could not find an apartment for a month, to my officemate Sonja for peace in the office, to Samira for being a strong woman with a red lipstick, to Evgenyi for staying in Linköping and to the skiing/snowboarding team: Spartak, Jolanta and Nisse.

I would like to mention other people at MAI that made it a great place to work and develop: Hans, Jesper, Theresa, Theresia, Monika, Joakim, Mikael L. and Johan.

I would like to acknowledge, my dad Krzysztof for asking me all those small crazy interesting questions about physics that I have always continued asking myself ever since.

Then, there is a kiss to Andrea, my super handsome Italian guy.

Oh! And I definitely should mention our 2 year-old kid Maja, who improved my time management, a lot.

List of Papers

- I A. Orlof, J. Ruseckas, I. V. Zozoulenko, *Effect of zigzag and armchair edges on the electronic transport in single-layer and bilayer graphene nanoribbons with defects*, Phys. Rev B **88**, 125409 (2013).
Author's contribution: Numerical simulations, preparation of most of the figures and big parts of the text.
- II A. Orlof, A. A. Shylau, I. V. Zozoulenko, *Electron-electron interactions in graphene field-induced quantum dots in a high magnetic field*, Phys. Rev. B **92**, 075431 (2015).
Author's contribution: Implementation of the numerical models, numerical calculations, analysis and discussion; writing of the paper draft.
- III V. Kozlov, S. Nazarov, A. Orlof, *Trapped modes supported by localized potentials in the zigzag graphene ribbon*, Comptes Rendus Mathematique 351 (1), 63-67 (2016).
Author's contribution: Contribution to the approach development and its analysis.
- IV V. Kozlov, S. Nazarov, A. Orlof, *Trapped modes in zigzag graphene nanoribbons*, (submitted).
Author's contribution: Contribution to the approach development, analysis, derivations and proofs; writing the paper draft.
- V V. Kozlov, S. Nazarov, A. Orlof, *Trapped modes in armchair graphene nanoribbons* (manuscript).
Author's contribution: Contribution to the approach development, analysis, derivations and proofs; writing the paper draft.
- VI F. Bentsson, A. Orlof, J. Thim, *Error Estimation for Eigenvalues of Unbounded Linear Operators and an Application to Energy Levels in Graphene Quantum Dots*, Numer. Funct. Anal. Optim. 38 (3), 293-305 (2017).
Author's contribution: Numerical calculations and analysis of the example in Graphene Quantum Dots.

Contents

Abstract	i
Populärvetenskaplig sammanfattning	iii
Acknowledgements	v
List of Papers	vii
Introduction	1
1 Introduction	3
2 Graphene	4
2.1 The discrete model	4
2.1.1 The graphene lattice	4
2.1.2 The reciprocal lattice	5
2.1.3 Brillouin Zone	6
2.1.4 Wavefunction	6
2.1.5 Bloch Theorem	8
2.1.6 Tight-binding model and the dispersion relation	8
2.1.7 Potential	9
2.2 The continuous model	10
2.3 The magnetic field	13
3 Graphene structures	15
3.1 Nanoribbons	15
3.1.1 Zigzag graphene nanoribbons	15
3.1.2 Armchair graphene nanoribbons	16
3.2 Bilayer graphene	18
3.3 Quantum dots	20
4 Transport and scattering in nanoribbons	21
4.1 The Landauer approach	21
4.2 Scattering in the discrete tight-binding model	21
4.2.1 The Green's function	22
4.2.2 The recursive Green's function technique	24
5 Electron-electron interactions	30
5.1 The many body problem	30
5.2 The independent electron approximation	30
5.3 The density functional theory	32
5.4 The Thomas Fermi approximation	33

6 Summary of the papers	35
6.1 Paper I	35
6.2 Paper II	35
6.3 Papers III and IV	35
6.4 Paper V	36
6.5 Paper VI	37
References	38
 Paper I	 41
 Paper II	 55
 Paper III	 65
 Paper IV	 73
 Paper V	 115
 Paper VI	 147

Introduction

1 Introduction

Andre Geim was a brilliant student that once won a contest for memorising a thousand-page chemistry dictionary. His experiment with the levitating frog won an Ig Nobel Prize for research that makes people laugh and then make them think. Straight after this prize, he started Friday seminars with his students directed to free form curiosity-driven research. During one of those meetings, he advised one of his PhD students to polish a piece of graphite to obtain the thinnest possible piece. After a few weeks the PhD student delivered the polished piece, which under a microscope was like a mountain of layers; however one of the fellows noticed a ball of scotch tape in the trash, covered with gray graphite. Geim took a piece of this scotch tape ball under the microscope to discover the thinnest pieces of graphite he had ever seen.

Since then, graphene gained a lot of attention due to its remarkable properties, such as [20, 23]

- remarkable thinness of only one atom (a million times thinner than a diameter of a human hair)
- very high electron mobility at rooms temperature, namely $200\,000 \frac{\text{cm}^2}{\text{Vs}}$, which is more than twice that of the highest mobility conventional semiconductors (silicon has $1\,400 \frac{\text{cm}^2}{\text{Vs}}$ and indium antimonide $77\,000 \frac{\text{cm}^2}{\text{Vs}}$);
- very high strength, with a Young's modulus of 1 TPa as for diamond and an intrinsic strength (maximum stress that material can withstand) of 130 GPa, so that it can sustain a weight of 2 tonnes focused on a pencil tip, before breaking;
- very high thermal conductivity, above $3000 \frac{\text{W}}{\text{mK}}$ (more than 7 times that of copper)
- high transparency, with optical transmittance of 97.7% (while window glass has 83%)
- impermeability to gases
- sustainment of extremely high densities of electric current (a million times higher than copper)

These properties are obtained in very high-quality samples and can vary strongly due to the edge influence, defects or external potentials. That is why this thesis is directed to check

- how quantum scattering in graphene nanoribbons is affected by edges, defects and external potentials
- how interaction influences graphene quantum dots.

In the next sections we introduce the basics of graphene [1, 3, 5, 9, 10, 16, 23, 22], graphene structures [4, 16, 18, 26], transport and scattering [6, 7, 11, 28, 29, 25] and interaction [3, 15, 17, 24] which are the background for the articles included in the thesis.

Figure 1: a) Graphene lattice consisting of two interpenetrating triangular lattices A (red) and B (blue). Yellow arrows represent the graphene primitive lattice vectors $\vec{a}_1$, $\vec{a}_2$ and the nearest-neighbour vectors $\vec{\tau}_1$, $\vec{\tau}_2$ and $\vec{\tau}_3$. A unit cell is indicated by the rhombus, it contains two orbitals at position (p, q) (referring to position $\mathbf{X}_{p,q}^A$ in lattice A and $\mathbf{X}_{p,q}^B$ in lattice B). b) Reciprocal lattice in the k -space. Yellow arrows represent the reciprocal lattice vectors $\vec{b}_1$ and $\vec{b}_2$. The First Brillouin Zone is within the yellow hexagon. The two indifferent corners of the Brillouin zone are called $\mathbf{K}$ and $\mathbf{K}'$.

2 Graphene

2.1 The discrete model

2.1.1 The graphene lattice

A graphene sheet is a hexagonal lattice of carbon atoms. From a crystallographical point of view, graphene has to be described as a Bravais lattice (a lattice of points that appears exactly the same from whichever point are viewed). This yields a graphene unit cell with two inequivalent carbon atoms and a lattice structure as a composition of two interpenetrating triangular lattices, called A and B (Figure 1 (a)). Every carbon atom has six electrons; two of them in the closed shell, the other four as valence electrons. Three of the valence electrons, one in s orbital and two in p orbitals, hybridise to sp^2 orbitals and bond with the three nearest neighbour electrons via strong σ -bonds (Figure 2). Those orbitals are situated in the graphene plane and create the hexagonal lattice (Figure 2). The last valence electron remains in its p orbital, perpendicular to graphene lattice and form weak π -bonds with its nearest neighbour p orbitals. The overlap of the p orbital with orbitals from next-nearest carbon atoms is significantly smaller. This leads to a tight-binding description of graphene with a crystalline structure of carbon atoms connected via σ -bonds and weakly bounded π electrons. This weakly bound π electrons account for all the unusual properties that graphene shows.

Let us now describe a direct lattice of graphene with the help of two primitive lattice

Figure 2: a) Hybridisation of the valence electron orbitals in graphene carbon atoms: three in plane sp^2 orbitals (in blue) and one perpendicular p_z orbital (in green). b) The sp^2 orbitals (blue) make the hexagonal graphene lattice, the remaining p_z orbitals (green) are out of the plane.

vectors (Figure 1 (a))

$$\vec{a}_1 = \left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right)a, \quad \vec{a}_2 = \left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)a, \quad a = \sqrt{3}a_{CC},$$

where a is the length of those vectors and $a_{CC} \approx 0.142[\text{nm}]$ is the distance between two nearest-neighbour carbon atoms. All the points in sublattices A and B lie in the position space $\mathbb{R}^2$ and are defined by the position vectors

$$\mathbf{X}_{p,q}^A = -\vec{\tau}_1 + p\vec{a}_1 + q\vec{a}_2,$$

$$\mathbf{X}_{p,q}^B = p\vec{a}_1 + q\vec{a}_2,$$

where p and q are integers and $\vec{\tau}_1$ is one of the nearest-neighbour vectors (Figure 1 (a))

$$\vec{\tau}_1 = \frac{a}{\sqrt{3}}(-1, 0), \quad \vec{\tau}_2 = \frac{a}{\sqrt{3}}\left(\frac{1}{2}, -\frac{\sqrt{3}}{2}\right), \quad \vec{\tau}_3 = \frac{a}{\sqrt{3}}\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right).$$

The nearest-neighbour vectors connect every point in sublattice B with its three nearest neighbours in sublattice A .

Any physical property that depends on $(x, y) \in \mathbb{R}^2$ is invariant under translation by primitive vectors $\vec{a}_1$ and $\vec{a}_2$.

The graphene unit cell contains two atoms and has an area $A_{\text{cell}} = \sqrt{3}a^2$ (rhombus in Figure 1 (a)).

2.1.2 The reciprocal lattice

A Fourier transform of an integrable function $f : \mathbb{R}^2 \rightarrow \mathbb{C}$ is defined as

$$\hat{f}(\vec{k}) = \iint_{-\infty}^{+\infty} f(\vec{x}) e^{-i\vec{x} \cdot \vec{k}} d\vec{x}, \quad \vec{x} = (x, y), \quad \vec{k} = (k_x, k_y).$$

The reciprocal lattice is a Fourier transform of a direct Bravais lattice and lies in the momentum space (k -space). The reciprocal lattice vectors (Figure 1 (b))

$$\vec{b}_1 = \left(\frac{2\pi}{\sqrt{3}a}, \frac{2\pi}{a} \right), \quad \vec{b}_2 = \left(\frac{2\pi}{\sqrt{3}a}, -\frac{2\pi}{a} \right)$$

are obtained from the direct lattice vectors and they fulfill $\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{i,j}$, $i, j = 1, 2$.

Any physical property that depends on (k_x, k_y) in the k -space is invariant under translation by reciprocal lattice vectors $\vec{b}_1$ and $\vec{b}_2$.

2.1.3 Brillouin Zone

A Wigner-Seitz cell is a region around a point that is closer to that point than to any other point of the lattice. The First Brillouin Zone is a Wigner-Seitz cell of the reciprocal lattice (yellow hexagon in Figure 1 (b)). From the periodicity of the k -space and the Bloch Theorem (Sect. 2.1.5) will follow that electrons wave functions can be defined with the help of a wave vector $\vec{k}$ from a k -space that lies in the First Brillouin Zone.

The six corners of this zone are called K points. Only two of them are inequivalent (within the nearest tight-binding model, that will be described later, Sect. 2.1.6 and Sect. 2.2), they are called $\mathbf{K}$ and $\mathbf{K}'$ (Figure 1 (b))

$$\mathbf{K} = \frac{1}{3}(\vec{b}_2 - \vec{b}_1) = \frac{4\pi}{3a}(0, -1), \quad \mathbf{K}' = \frac{1}{3}(\vec{b}_1 - \vec{b}_2) = \frac{4\pi}{3a}(0, 1),$$

2.1.4 Wavefunction

Having a graphene lattice, we consider all possible electronic configurations in that lattice. Namely, we can have no electrons (vacuum state), one electron that occupies a certain position, two electrons that occupy two different positions and so on. Assuming that electrons are indifferent and not-interacting, all the possible states can be described with the use of the Fock-space [19]

$$\mathcal{F} = \bigoplus_{j=0}^{\infty} (\mathbb{H}^{\wedge j}) = \mathbb{C} \oplus \mathbb{H} \oplus (\mathbb{H} \wedge \mathbb{H}) \oplus \dots,$$

where $\mathbb{C}$ contains zero particle states with a vacuum state $1 =: |0\rangle$ (being one of the wedge product); $\mathbb{H}$ is a Hilbert space of single particle states (orbitals); $\mathbb{H} \wedge \mathbb{H}$ is a wedge product of two one particle spaces $\mathbb{H}$ etc. The basis of the single particle states $\mathbb{H}$ can be denoted as $|1\rangle, |2\rangle, |3\rangle, \dots$, where $|i\rangle$ is a state of one electron at position $i = (p, q)$. A basis used for the whole Fock space $\mathcal{F}$ is the occupancy number basis with antisymmetric elements $|n_1, n_2, \dots, n_k\rangle$, where $n_i = 0, 1$ denotes the number of particles in state $|i\rangle$. For example a state of one electron at position one and one at position two is

$$|1_1, 1_2\rangle = |1\rangle \wedge |2\rangle = \frac{|1\rangle \otimes |2\rangle - |2\rangle \otimes |1\rangle}{\sqrt{2}},$$

the wedge product reflects the asymmetry of states under the exchange of two particles. The inner product in space $\mathcal{F}$ is the sum of the inner products in all the composite Hilbert spaces $\mathbb{H}^{\wedge j}$, $j = 0, 1, \dots$

A wavefunction of an electron in graphene is a superposition of one-particle states

$$|\psi\rangle = \sum_i \zeta_i^A |i\rangle + \sum_i \zeta_i^B |i\rangle. \quad (2.1)$$

where a complex number ζ_i^A (ζ_i^B) is the probability amplitude of finding the electron at position $\mathbf{X}_{p,q}^A$ ($\mathbf{X}_{p,q}^B$). This wavefunction can be written with the help of creation and annihilation operators. The creation (annihilation) operators a_i , b_i ($a_i^\dagger$, $b_i^\dagger$) create (annihilate) an electron on site $\mathbf{X}_{p,q}^A$ (for a_i , $a_i^\dagger$) and $\mathbf{X}_{p,q}^B$ (for b_i , $b_i^\dagger$) with $i = (p, q)$, namely

$$a_i^\dagger : \mathcal{F} \rightarrow \mathcal{F}, \quad a_i : \mathcal{F} \rightarrow \mathcal{F}.$$

The operator $a_i^\dagger$ acting on a n -particle state $|\Psi\rangle \in \mathcal{F}$, inserts a single particle $|i\rangle$ in $n+1$ positions anti-symmetrically and introduces a factor $\frac{1}{\sqrt{n+1}}$. The operator a_i performs in a reverse way and acting on a n -particle state $|\Psi\rangle \in \mathcal{F}$, deletes a single particle state $|i\rangle$ from n positions anti-symmetrically and introduces a factor $\frac{1}{\sqrt{n}}$. For example

$$a_2^\dagger |1\rangle = \frac{|1\rangle \otimes |2\rangle - |2\rangle \otimes |1\rangle}{\sqrt{2}},$$

$$a_1^\dagger |1\rangle = 0,$$

where the collapse of the wavefunction in last equality is a consequence of the Pauli Principle, which forbids two identical electrons to occupy the same state. Annihilation operator $a_i^\dagger$ ($b_i^\dagger$) is a Hermitian conjugate of the creation operator a_i (b_i), the operators fulfil the anti-commutation relations

$$\{a_i, a_j^\dagger\} = \delta_{ij} \mathcal{I},$$

$$\{a_i, a_j\} = \{a_i^\dagger, a_j^\dagger\} = 0,$$

and form a $*$ -algebra or, when completed, a C^* -algebra.

In particular, for graphene we use only single particle states and the following properties of creation/annihilation operators

$$a_i^\dagger |0\rangle = |i\rangle,$$

$$a_i |i\rangle = |0\rangle, \quad a_i |j\rangle = 0, \quad a_i |0\rangle = 0, \quad i \neq j,$$

and a states $|0\rangle, |j\rangle$ with j that runs over lattice positions.

Now, the electron wave function (2.1) can be written as

$$|\psi\rangle = \sum_i \left(\zeta_i^A a_i^\dagger + \zeta_i^B b_i^\dagger \right) |0\rangle. \quad (2.2)$$

2.1.5 Bloch Theorem

From the translational symmetry of the direct lattice follows the Bloch theorem. It states that energy eigenstates for an electron in a crystal can be written as Bloch waves, that is

$$\langle \vec{x} | \psi \rangle = \psi(\vec{x}) = u(\vec{x}) e^{i\vec{k} \cdot \vec{x}}, \quad (2.3)$$

where $\vec{x} \in \mathbb{R}^2$, $\vec{k}$ is from the k -space and a function $u(\vec{x})$ has the periodicity of the direct lattice

$$u(\vec{x}) = u(\vec{x} + p\vec{a}_1 + q\vec{a}_2),$$

with integers p, q .

Note that due to the translational invariance in the k -space, a wavefunction with $\vec{k}$ (crystal momentum) (2.3) describes electron, as well as the one with $\vec{k}' = \vec{k} + \vec{\kappa}$ with $\vec{\kappa}$ is from the reciprocal lattice. That is why $\vec{k}$ is called a crystal momentum, not a particle momentum, as the latter has to be a conserved quantity.

Again, from the translational invariance follows that a wavefunction in the Bloch form can be defined with the use of a wavevector from the First Brillouin Zone only.

We can express our wavefunction (2.2) with the help of the Bloch theorem getting

$$\psi(\mathbf{X}_{p,q}^{A(B)}) = \langle \mathbf{X}_{p,q}^{A(B)} | \psi \rangle = \zeta_{p,q}^{A(B)} = \psi^{A(B)} e^{i\vec{k} \cdot \mathbf{X}_{p,q}^{A(B)}}. \quad (2.4)$$

2.1.6 Tight-binding model and the dispersion relation

One can consider the tight-binding nearest-neighbour model for a single-electron in graphene with its Hamiltonian given by

$$\mathcal{H} = -t \sum_{i,\Delta} (a_i^\dagger b_{i+\Delta} + b_{i+\Delta}^\dagger a_i) = -t \sum_{p,q} (a_{p,q}^\dagger b_{p,q} + a_{p,q}^\dagger b_{p,q-1} + a_{p,q}^\dagger b_{p-1,q} + \text{h.c.}), \quad (2.5)$$

where Δ runs over nearest neighbours of cell i and $t = 2.77\text{eV}$ is the nearest-neighbour hopping integral.

Now, the Schrödinger equation reads

$$\mathcal{H}|\psi\rangle = E|\psi\rangle.$$

Using (2.2) with $i = (p, q)$, we can calculate $\langle 0 | a_{p,q} \mathcal{H} | \psi \rangle$ and $\langle 0 | b_{p,q} \mathcal{H} | \psi \rangle$, which give us the difference equations

$$-t \sum_{j=1}^3 \psi(\mathbf{X}_{p,q}^A - \vec{\tau}_j) = E \psi(\mathbf{X}_{p,q}^A), \quad (2.6)$$

$$-t \sum_{j=1}^3 \psi(\mathbf{X}_{p,q}^B + \vec{\tau}_j) = E \psi(\mathbf{X}_{p,q}^B). \quad (2.7)$$

Note that $\psi(\mathbf{X}_{p,q}^A - \vec{\tau}_1) = \zeta_{p,q}^B$, $\psi(\mathbf{X}_{p,q}^A - \vec{\tau}_2) = \zeta_{p,q-1}^B$, $\psi(\mathbf{X}_{p,q}^A - \vec{\tau}_3) = \zeta_{p-1,q}^B$, etc.

According to the Bloch Theorem (Sec. 2.1.5) we have (2.4) and

$$\psi(\mathbf{X}_{p,q}^B + \vec{\tau}_j) = \psi^A e^{i\vec{k}(\mathbf{X}_{p,q}^B + \vec{\tau}_j)}, \quad \psi(\mathbf{X}_{p,q}^A - \vec{\tau}_j) = \psi^B e^{i\vec{k}(\mathbf{X}_{p,q}^A - \vec{\tau}_j)} \quad j = 1, 2, 3. \quad (2.8)$$

Using this Bloch form of the wave function in (2.6), (2.7), we get

$$-t\psi^B \sum_{j=1}^3 e^{-i\vec{k}\vec{\tau}_j} = E\psi^A,$$

$$-t\psi^A \sum_{j=1}^3 e^{i\vec{k}\vec{\tau}_j} = E\psi^B,$$

now, defining

$$\phi(\vec{k}) = \sum_{j=1}^3 e^{-i\vec{k}\vec{\tau}_j}$$

enables us to write

$$\hat{\mathcal{H}} \begin{pmatrix} \psi^A \\ \psi^B \end{pmatrix} = E \begin{pmatrix} \psi^A \\ \psi^B \end{pmatrix}, \quad \hat{\mathcal{H}} = \begin{pmatrix} 0 & -t\phi(\vec{k}) \\ -t\phi^*(\vec{k}) & 0 \end{pmatrix}.$$

and determine the energies as $\det(\hat{\mathcal{H}} - \mathcal{J}E) = 0$, which gives

$$E^2 = t^2 |\phi|^2$$

so that the dispersion relation becomes

$$E(k_x, k_y) = \pm t \sqrt{1 + 4 \cos^2\left(\frac{\sqrt{3}}{2} a_{cc} k_y\right) + 4 \cos\left(\frac{\sqrt{3}}{2} a_{cc} k_y\right) \cos\left(\frac{3}{2} a_{cc} k_x\right)}.$$

and it is visualised in Figure 3.

2.1.7 Potential

An external potential describes

- defects: vacancies, adatoms, Coulomb impurities, wrinkles, ripples and other
- external electric field.

Depending on its nature it can be modelled as a short or long range one.

It results in the onsite energy, which can be incorporated in the Tight-Binding Hamiltonian (2.5) by additional term

$$\mathcal{P}_0 = \sum_i (\mathcal{P}_i^A a_i^\dagger a_i + \mathcal{P}_i^B b_i^\dagger b_i),$$

Figure 3: a) Dispersion relation in the discrete model and b) its projection on the k_x, k_y plane, with six K -points with zero energy shown by minima in dark blue.

where $\mathcal{P}_i^A = \mathcal{P}(\mathbf{X}_{p,q}^A)$, $\mathcal{P}_i^B = \mathcal{P}(\mathbf{X}_{p,q}^B)$ is the magnitude of the potential on site i in lattice A, B . The inclusion of such a potential leads to new difference equations

$$-t \sum_{j=1}^3 \psi(\mathbf{X}_{p,q}^A - \vec{\tau}_j) = (E - \mathcal{P}(\mathbf{X}_{p,q}^A)) \psi(\mathbf{X}_{p,q}^A), \quad (2.9)$$

$$-t \sum_{j=1}^3 \psi(\mathbf{X}_{p,q}^B + \vec{\tau}_j) = (E - \mathcal{P}(\mathbf{X}_{p,q}^B)) \psi(\mathbf{X}_{p,q}^B). \quad (2.10)$$

2.2 The continuous model

The continuous model is derived from the discrete tight-binding model within the low-energy approximation. In the tight-binding model, the dispersion relation has six minima within the first Brillouin Zone (Figure 3). Only two of those minima are inequivalent, while the remaining four lead to the equivalent envelope wave functions. In this section, we derive the differential equations that describe the electron dynamics close to the two inequivalent minima called $\mathbf{K}$ and $\mathbf{K}'$ [16].

Let us assume that the wavevector can be written in the form

$$\psi(\mathbf{X}^A) = e^{i\mathbf{K} \cdot \mathbf{X}^A} u(\mathbf{X}^A) - i e^{i\mathbf{K}' \cdot \mathbf{X}^A} u'(\mathbf{X}^A), \quad (2.11)$$

$$\psi(\mathbf{X}^B) = -i e^{i\mathbf{K} \cdot \mathbf{X}^B} v(\mathbf{X}^B) + e^{i\mathbf{K}' \cdot \mathbf{X}^B} v'(\mathbf{X}^B). \quad (2.12)$$

For simplification, we omit the index (p, q) in (2.11), (2.12) and (2.9), (2.10) as this relations hold for any (p, q) .

Inserting functions (2.11) and (2.12) into (2.9) and (2.10) give

$$\begin{aligned}
& -t \sum_{j=1}^3 \left(-i e^{i\mathbf{K} \cdot (\mathbf{X}^A - \vec{r}_j)} v(\mathbf{X}^A - \vec{r}_j) + e^{i\mathbf{K}' \cdot (\mathbf{X}^A - \vec{r}_j)} v'(\mathbf{X}^A - \vec{r}_j) \right) \\
& = \left(E - \mathcal{P}(\mathbf{X}^A) \right) \left(e^{i\mathbf{K} \cdot \mathbf{X}^A} u(\mathbf{X}^A) - i e^{i\mathbf{K}' \cdot \mathbf{X}^A} u'(\mathbf{X}^A) \right)
\end{aligned} \tag{2.13}$$

$$\begin{aligned}
& -t \sum_{j=1}^3 \left(e^{i\mathbf{K} \cdot (\mathbf{X}^B + \vec{r}_j)} u(\mathbf{X}^B + \vec{r}_j) - i e^{i\mathbf{K}' \cdot (\mathbf{X}^B + \vec{r}_j)} u'(\mathbf{X}^B + \vec{r}_j) \right) \\
& = \left(E - \mathcal{P}(\mathbf{X}^B) \right) \left(-i e^{i\mathbf{K} \cdot \mathbf{X}^B} v(\mathbf{X}^B) + e^{i\mathbf{K}' \cdot \mathbf{X}^B} v'(\mathbf{X}^B) \right).
\end{aligned} \tag{2.14}$$

To pass from the discrete positions $\mathbf{X}^A$ and $\mathbf{X}^B$ to a continuous variable $\mathbf{x} = (x, y)$ and get

$$\psi(\mathbf{X}^A) = \psi_A(\mathbf{x}), \quad \psi(\mathbf{X}^B) = \psi_B(\mathbf{x}),$$

let us define a smoothening real-value function $g(\mathbf{x})$, which

- is centred at $\mathbf{x}$,
- decays rapidly within few lattice-constant distance from the centre,
- $\sum_{\mathbf{X}^{A(B)}} g(\mathbf{x} - \mathbf{X}^{A(B)}) = 1$,
- $\int_{\Omega} g(\mathbf{x} - \mathbf{X}^{A(B)}) d\mathbf{x} = A_{\text{cell}}$ (interpreted as one electron in lattice A and one in lattice B per one unit cell), where Ω is area of the whole graphene sheet,
- $\sum_{\mathbf{X}^{A(B)}} g(\mathbf{x} - \mathbf{X}^{A(B)}) e^{i(\mathbf{K}' - \mathbf{K}) \cdot \mathbf{X}^{A(B)}} \approx 0$,
- $f(\mathbf{x}) g(\mathbf{x} - \mathbf{X}^{A(B)}) \approx f(\mathbf{X}^{A(B)}) g(\mathbf{x} - \mathbf{X}^{A(B)})$, where f is any function.

Multiplying equation (2.13) by $g(\mathbf{x} - \mathbf{X}^A) e^{-i\mathbf{K} \cdot \mathbf{X}^A}$, summing up over $\mathbf{X}^A$ and using the properties of function $g(\mathbf{x})$, we arrive at

$$-t \sum_{j=1}^3 -i e^{-i\mathbf{K} \cdot \vec{r}_j} v(\mathbf{x} - \vec{r}_j) \approx E u(\mathbf{x}) - \mathcal{P}_A(\mathbf{x}) u(\mathbf{x}) + i \tilde{\mathcal{P}}_A(\mathbf{x}) u'(\mathbf{x}), \tag{2.15}$$

where

$$\mathcal{P}_A(\mathbf{x}) = \sum_{\mathbf{X}^A} \mathcal{P}(\mathbf{X}^A) g(\mathbf{x} - \mathbf{X}^A), \quad \tilde{\mathcal{P}}_A(\mathbf{x}) = \sum_{\mathbf{X}^A} \mathcal{P}(\mathbf{X}^A) e^{i(\mathbf{K}' - \mathbf{K}) \cdot \mathbf{X}^A} g(\mathbf{x} - \mathbf{X}^A).$$

Now, we use the expansion

$$v(\mathbf{x} - \vec{r}_j) \approx v(\mathbf{x}) - \vec{r}_j \cdot (\partial_x, \partial_y) v(\mathbf{x}), \tag{2.16}$$

which is valid for low energies only ($a_{CC} \rightarrow 0$, $|\vec{r}_j| = a_{CC}$). As

$$\sum_j e^{-i\mathbf{K}\cdot\vec{\tau}_j} = 1 + e^{-i\frac{2\pi}{3}} + e^{i\frac{2\pi}{3}} = 0, \quad (2.17)$$

$$\sum_j e^{-i\mathbf{K}\cdot\vec{\tau}_j} \vec{\tau}_j \cdot (\partial_x, \partial_y) = \frac{\sqrt{3}a}{2} (-\partial_x + i\partial_y), \quad (2.18)$$

we get that equation (2.15) becomes

$$\frac{\sqrt{3}a}{2} t (i\partial_x + \partial_y) v(\mathbf{x}) \approx Eu(\mathbf{x}) - \mathcal{P}_A(\mathbf{x})u(\mathbf{x}) + i\tilde{\mathcal{P}}_A(\mathbf{x})u'(\mathbf{x}). \quad (2.19)$$

Analogously, multiplying equation (2.14) by $ig(\mathbf{x} - \mathbf{X}^B)e^{-i\mathbf{K}\cdot\mathbf{X}^B}$, summing up over $\mathbf{X}^B$ and using properties similar to (2.16), (2.17), (2.18), we get

$$\frac{\sqrt{3}a}{2} t (i\partial_x - \partial_y) u(\mathbf{x}) \approx Ev(\mathbf{x}) - \mathcal{P}_B(\mathbf{x})v(\mathbf{x}) - i\tilde{\mathcal{P}}_B(\mathbf{x})v'(\mathbf{x}), \quad (2.20)$$

where

$$\mathcal{P}_B(\mathbf{x}) = \sum_{\mathbf{X}^B} \mathcal{P}(\mathbf{X}^B) g(\mathbf{x} - \mathbf{X}^B), \quad \tilde{\mathcal{P}}_B(\mathbf{x}) = \sum_{\mathbf{X}^B} \mathcal{P}(\mathbf{X}_B) e^{i(\mathbf{K}' - \mathbf{K})\cdot\mathbf{X}^B} g(\mathbf{x} - \mathbf{X}^B).$$

Multiplying equation (2.13) by $ig(\mathbf{x} - \mathbf{X}_A)e^{-i\mathbf{K}'\cdot\mathbf{X}_A}$ and summing up over $\mathbf{X}_A$, we arrive at

$$\frac{\sqrt{3}a}{2} t (-i\partial_x + \partial_y) v'(\mathbf{x}) \approx Eu'(\mathbf{x}) - \mathcal{P}_A(\mathbf{x})u'(\mathbf{x}) - i\tilde{\mathcal{P}}_A^*(\mathbf{x})u(\mathbf{x}). \quad (2.21)$$

And finally multiplying equation (2.14) by $g(\mathbf{x} - \mathbf{X}_B)e^{-i\mathbf{K}'\cdot\mathbf{X}_B}$ and summing up over $\mathbf{X}_B$, leads to

$$\frac{\sqrt{3}a}{2} t (-i\partial_x - \partial_y) u'(\mathbf{x}) \approx Ev'(\mathbf{x}) - \mathcal{P}_B(\mathbf{x})v'(\mathbf{x}) + i\tilde{\mathcal{P}}_B^*(\mathbf{x})v(\mathbf{x}). \quad (2.22)$$

For simplicity, let us define the quantity $\gamma = \frac{\sqrt{3}a}{2} t = v_F \hbar$, where $v_F \approx 10^6 \frac{m}{s}$ is the Fermi velocity of electrons in graphene. Now (2.19), (2.20), (2.21) and (2.22) can be written in the matrix form and we arrive at the Dirac equation

$$D \begin{pmatrix} u \\ v \\ u' \\ v' \end{pmatrix} \approx E \begin{pmatrix} u \\ v \\ u' \\ v' \end{pmatrix}, \quad (2.23)$$

$$D = \begin{pmatrix} \mathcal{P}_A(\mathbf{x}) & \gamma(i\partial_x + \partial_y) & -i\tilde{\mathcal{P}}_A(\mathbf{x}) & 0 \\ \gamma(i\partial_x - \partial_y) & \mathcal{P}_B(\mathbf{x}) & 0 & i\tilde{\mathcal{P}}_B(\mathbf{x}) \\ i\tilde{\mathcal{P}}_B^*(\mathbf{x}) & 0 & \mathcal{P}_A(\mathbf{x}) & \gamma(-i\partial_x + \partial_y) \\ 0 & -i\tilde{\mathcal{P}}_B^*(\mathbf{x}) & \gamma(-i\partial_x - \partial_y) & \mathcal{P}_B(\mathbf{x}) \end{pmatrix}. \quad (2.24)$$

Equation (2.23) is defined as a continuous Dirac model and so from now on, we will write equality sign in (2.23).

When the potential is assumed to be of long-range type, then [2] $\tilde{\mathcal{P}}_A(\mathbf{x}) = \tilde{\mathcal{P}}_B(\mathbf{x}) = 0$ and $\mathcal{P}(\mathbf{x}) := \mathcal{P}_A(\mathbf{x}) = \mathcal{P}_B(\mathbf{x})$.

Finally, when there is no potential, $\mathcal{P}(\mathbf{x}) = 0$, the Dirac operator (2.23) becomes

$$D = \begin{pmatrix} 0 & \gamma(i\partial_x + \partial_y) & 0 & 0 \\ \gamma(i\partial_x - \partial_y) & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma(-i\partial_x + \partial_y) \\ 0 & 0 & \gamma(-i\partial_x - \partial_y) & 0 \end{pmatrix} \quad (2.25)$$

and using the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \vec{\sigma} = (\sigma_x, \sigma_y),$$

we can write (2.23) as

$$D = \begin{pmatrix} D_K & 0 \\ 0 & D_{K'} \end{pmatrix}, \quad D_K = \gamma i \vec{\sigma} \cdot \nabla, \quad D_{K'} = \gamma i \vec{\sigma}^* \cdot \nabla. \quad (2.26)$$

Taking the Fourier transform of

$$D_K \begin{pmatrix} u \\ v \end{pmatrix} = E \begin{pmatrix} u \\ v \end{pmatrix} \quad (2.27)$$

and $D_{K'} \begin{pmatrix} u' \\ v' \end{pmatrix} = E \begin{pmatrix} u' \\ v' \end{pmatrix}$ that changes the variable from $\vec{x}$ to $\vec{p} = (p_x, p_y)$ or equivalently assuming that $\vec{k} = \mathbf{K} + \vec{p}$ close to K point and $\vec{k} = \mathbf{K}' + \vec{p}$ close to K', we get

$$E = \pm \gamma |\vec{p}|,$$

what shows that in the continuous model the dispersion relation is linear.

2.3 The magnetic field

The addition of a perpendicular magnetic field changes the continuous spectrum into series of Landau Levels. The magnetic field is incorporated into the Dirac Hamiltonian (2.25) by the change of momentum [19]

$$\hbar \vec{p} \rightarrow \hbar \vec{p} - e \vec{A}, \quad i \nabla \rightarrow i \nabla + \frac{e}{\hbar} \vec{A}, \quad (2.28)$$

where $-e$ is the electrons charge and $\vec{A}$ is the magnetic vector potential. One of the magnetic vector potentials that give rise to magnetic field perpendicular to graphene plane $\vec{B} = (0, 0, 1)$ is

$$\vec{A} = (A_x, A_y) = (-By, 0), \quad (2.29)$$

as $\vec{B} = \nabla \times \vec{A}$ (with $A_z = 0$). As the equations for $\mathbf{K}$ and $\mathbf{K}'$ valleys are separated in pristine graphene, we consider the $\mathbf{K}$ valley only, then

$$(i\partial_x + \partial_y)(i\partial_x - \partial_y)u = \left(\frac{E}{\hbar v_F}\right)^2 u,$$

$$v = \frac{\hbar v_F}{E}(i\partial_x - \partial_y).$$

Now applying the momentum change (2.28), we get

$$(i\partial_x - \frac{eB}{\hbar}y + \partial_y)(i\partial_x - \frac{eB}{\hbar}y - \partial_y)u = \left(\frac{E}{\hbar v_F}\right)^2 u, \quad (2.30)$$

$$v = \frac{\hbar v_F}{E}(i\partial_x - \frac{eB}{\hbar}y - \partial_y).$$

Assuming translational symmetry in the x variable allows us to assume

$$\begin{pmatrix} u(x, y) \\ v(x, y) \end{pmatrix} = e^{ip_x x} \begin{pmatrix} U(y) \\ V(y) \end{pmatrix},$$

that inserted into (2.30) and simplified gives

$$[-\partial_y^2 + (p_x + \frac{y}{l_B^2})^2]U(y) = \left(\left(\frac{E}{\hbar v_F}\right)^2 + \frac{1}{l_B^2}\right)U(y),$$

where $l_B = \sqrt{\frac{\hbar}{eB}}$ is the magnetic length. Now changing the variable to $\zeta = l_B p_x + \frac{y}{l_B}$, the last equation becomes

$$[-\partial_\zeta^2 + \zeta^2]U(\zeta) = \mathcal{E}U(\zeta), \quad \mathcal{E} = \left(\left(\frac{l_B E}{\hbar v_F}\right)^2 + 1\right),$$

and can be identified with the equation for the harmonic oscillator. Energies of such a system are called Landau Levels and are

$$\mathcal{E} = 2n + 1, \quad n = 0, 1, \dots$$

so

$$E = \pm \frac{\hbar v_F}{l_B} \sqrt{2n}, \quad n = 0, 1, \dots \quad (2.31)$$

with corresponding wavefunctions

$$U_n(\zeta) = e^{-\frac{\zeta^2}{2}} H_n(\zeta),$$

where H_n is the n -th order Hermite polynomial. Finally, the two component wave function corresponding to the n -th Landau Level is

$$u_n(x, y) = e^{ip_x x} \begin{pmatrix} U_n(l_B p_x + \frac{y}{l_B}) \\ U_{n-1}(l_B p_x + \frac{y}{l_B}) \end{pmatrix},$$

and describes a free electron.

The Landau Levels for two dimensional electron gas are equidistantly separated, differently The Landau Levels for graphene are not equally separated (2.31).

Figure 4: a) Zigzag nanoribbon, the width L is for the continuous model, for the discrete one the width $\tilde{L}$ is smaller by $a_{CC} = \frac{\sqrt{3}a}{3}$ b) Zigzag dispersion relation $E[t]$ vs $k_y[a]$ for a nanoribbon with $L = 11\sqrt{3}a$ $((11 + \frac{1}{3})\sqrt{3}a)$. Green curves are from tight-binding model and purple for continuous one.

3 Graphene structures

3.1 Nanoribbons

Graphene nanoribbons are divided into two groups according to their edge type: zigzag and armchair.

3.1.1 Zigzag graphene nanoribbons

The boundary value problem for zigzag nanoribbons is (2.23), (2.25) with the boundary conditions (Figure 4) [4]

$$\psi_A(0, y) = 0, \quad \psi_B(L, y) = 0$$

that according to definitions (2.11), (2.12), translate into

$$u(0, y) = 0, \quad u'(0, y) = 0, \quad v(L, y) = 0, \quad v'(L, y) = 0. \quad (3.1)$$

These boundary conditions separate (2.23), (2.25) into two systems, one close to the $\mathbf{K}$ and the other close to the $\mathbf{K}'$ valley, let us consider one of them (close to the $\mathbf{K}'$ valley)

$$D \begin{pmatrix} u' \\ v' \end{pmatrix} = E \begin{pmatrix} u' \\ v' \end{pmatrix}, \quad D = \gamma \begin{pmatrix} 0 & -i\partial_x + \partial_y \\ -i\partial_x - \partial_y & 0 \end{pmatrix} \quad (3.2)$$

Considering the nanoribbons geometry, let us assume the exponential form of the solution¹

$$(u'(x, y), v'(x, y)) = e^{ip_y y} (U'(x), V'(x)), \quad (3.3)$$

and substitute it into (3.2), (3.1), what gives

$$\begin{cases} -\mathcal{U}_{xx} = (\omega^2 - p_y^2) \mathcal{U}, & \mathcal{U}(0) = 0, & \mathcal{U}_x(L) = -p_y \mathcal{U}(L) \\ \mathcal{V} = \frac{1}{\omega} (-i \mathcal{U}_x - i p_y \mathcal{U}) \end{cases} \quad (3.4)$$

with $\omega = \frac{E}{\gamma}$. Consider two cases. First let's assume that $p_y^2 = \omega^2$. Then there exists an exponential solution only for $p_y = -\frac{1}{L}$ and it has the following form

$$\mathcal{U}(x) = -\frac{1}{L} x, \quad \mathcal{V}(x) = \frac{i}{L\omega} (1 - \frac{x}{L}). \quad (3.5)$$

Let's consider the second case and assume $p_y^2 \neq \omega^2$. Then the solution to (3.4) is given by

$$(\mathcal{U}(x), \mathcal{V}(x)) = \left(\sin(p_x x), \pm i \sin(p_x (x - L)) \right), \quad (3.6)$$

with

$$\frac{\sin(p_x L)}{p_x} = \pm \frac{1}{\omega}, \quad p_y = -p_x \cot(p_x L). \quad (3.7)$$

Note that $p_x^2 + p_y^2 = \omega^2$. For more detailed analysis look at the article III and IV. The dispersion relation is shown in Figure 4 (violet) and compared with the result for the discrete case (green, from formulas (8), (10) and (12) in article I).

3.1.2 Armchair graphene nanoribbons

The boundary value problem for armchair nanoribbons is (2.23), (2.25) with the boundary conditions (Figure 5) [4]

$$\psi_A(x, 0) = 0, \quad \psi_B(x, 0) = 0, \quad \psi_A(x, L) = 0, \quad \psi_B(x, L) = 0,$$

that according to the definitions (2.11), (2.12), become

$$u(x, 0) - i u'(x, 0) = 0, \quad -i v(x, 0) + v'(x, 0) = 0, \quad (3.8)$$

$$e^{-i2\pi L} u(x, L) - i u'(x, L) = 0, \quad -i e^{-i2\pi L} v(x, L) + v'(x, L) = 0. \quad (3.9)$$

Differently than for zigzag, the boundary conditions couple K and K' valleys so that the problem cannot be treated separately for every valley.

To find the wavefunctions that solve the system (2.23), (2.25), let us assume the exponential form²

¹Within the notation in Article IV, λ corresponds to scaled $-p_y$ and κ to scaled p_x .

²Within the notation in Article V, λ corresponds to scaled p_x and κ to scaled p_y .

Figure 5: a) Armchair nanoribbon, the width L is for the continuous model, for the discrete one the width $\tilde{L}$ is smaller by a . b) Armchair dispersion relation $E[t]$ vs $k_x[a]$ for a nanoribbon with $L = 18a$. Green curves are from tight-binding model and purple for continuous one.

$$(u(x, y), v(x, y), u'(x, y), v'(x, y)) = e^{ip_x x} (U(y), V(y), U'(y), V'(y)). \quad (3.10)$$

After insertion to (2.23), (2.25) with (3.8), (3.9), we get

$$\begin{cases} -\mathcal{U}_{yy} = (\omega^2 - p_x^2) \mathcal{U}, & -\mathcal{U}'_{yy} = (\omega^2 - p_x^2) \mathcal{U}' \\ \mathcal{V} = \frac{1}{\omega} (-p_x \mathcal{U} - \mathcal{U}_y), & \mathcal{V}' = \frac{1}{\omega} (p_x \mathcal{U}' - \mathcal{U}'_y), \\ \mathcal{U}(0) - i\mathcal{U}'(0) = 0, & -i\mathcal{V}(0) + \mathcal{V}'(0) = 0 \\ e^{-i2\pi L} \mathcal{U}(L) - i\mathcal{U}'(L) = 0, & -ie^{-i2\pi L} \mathcal{V}(L) + \mathcal{V}'(L) = 0. \end{cases} \quad (3.11)$$

If $p_x^2 = \omega^2$, then problem (3.11) has a non-trivial solution only when L is a natural number. In this case

$$(u(x, y), v(x, y), u'(x, y), v'(x, y)) = e^{\pm i\omega x} (1, \mp 1, -i, \mp i) \quad (3.12)$$

and there is no power exponential solution.

Now if $p_x^2 \neq \omega^2$, then the exponential solutions are

$$(\mathcal{U}(y), \mathcal{V}(y), \mathcal{U}'(y), \mathcal{V}'(y)) = (e^{ip_y y}, -\frac{p_x + ip_y}{\omega} e^{ip_y y}, -ie^{-ip_y y}, -\frac{i(p_x + ip_y)}{\omega} e^{-ip_y y}), \quad (3.13)$$

with

$$p_x = \pm \sqrt{\omega^2 - p_y^2}, \quad p_y = \pi + \frac{\pi j}{L}, \quad j = 0, \pm 1, \pm 2, \dots \quad (3.14)$$

Note that $p_x^2 + p_y^2 = \omega^2$. For a more detailed analysis look at article V. The dispersion relation is shown in Figure 5 (violet) and compared with the result for the discrete case (green, from formulas (8), (10) and (11) in article number I).

3.2 Bilayer graphene

Bilayer graphene consists of two layers of monolayer graphene. The upper layer is composed of two interpenetrating lattices A_1 and B_1 and the lower layer of A_2 and B_2 (Figure 6). The upper layer is shifted with respect to the lower one by a vector $[a_{CC}, 0]$ so that the elements of lattice A_1 are exactly above those from lattice A_2 . The hopping parameter between those aligned elements is $\gamma_1 = 0.39[\text{eV}]$. The second strongest hopping interaction between two layers is $\gamma_3 = 0.315[\text{eV}]$ and it describes the hopping between nearest-neighbour elements from lattices B_1 and B_2 .

Now, we can write the tight binding Hamiltonian for a single electron in bilayer graphene [18] as:

$$\begin{aligned} \mathcal{H} = & -t \sum_{i,l=1,2,\Delta} (a_{l,i}^\dagger b_{l,i+\Delta} + b_{l,i+\Delta}^\dagger a_{l,i}) \\ & -\gamma_1 \sum_i (a_{1,i}^\dagger a_{2,i} + a_{2,i}^\dagger a_{1,i}) - \gamma_3 \sum_i (b_{1,i}^\dagger b_{2,i} + b_{2,i}^\dagger b_{1,i}), \end{aligned} \quad (3.15)$$

where Δ runs over the nearest neighbours of cell $i = (p, q)$ within one layer and $a_{l,i}^\dagger$, $(a_{l,i})$, $b_{l,i}^\dagger$, $(b_{l,i})$ are creation/annihilation operators, that create/annihilate an electron in cell i that belong to sublattices A_l or B_l respectively. To find the bilayer graphene dispersion relation, we write its function in the Bloch form

$$\psi(\mathbf{X}_{p,q}^{B_1} + \vec{\tau}_j) = \psi^{A_1} e^{i\vec{k}(\mathbf{X}_{p,q}^{B_1} + \vec{\tau}_j)}, \quad \psi(\mathbf{X}_{p,q}^{A_1} - \vec{\tau}_j) = \psi^{B_1} e^{i\vec{k}(\mathbf{X}_{p,q}^{A_1} - \vec{\tau}_j)} \quad (3.16)$$

$$\psi(\mathbf{X}_{p,q}^{A_2} + \vec{\tau}_j) = \psi^{B_2} e^{i\vec{k}(\mathbf{X}_{p,q}^{A_2} + \vec{\tau}_j)}, \quad \psi(\mathbf{X}_{p,q}^{B_2} - \vec{\tau}_j) = \psi^{A_2} e^{i\vec{k}(\mathbf{X}_{p,q}^{B_2} - \vec{\tau}_j)} \quad (3.17)$$

where $\mathbf{X}_{p,q}^{A_l}$ ($\mathbf{X}_{p,q}^{B_l}$) is the position of an electron orbital in cell (p, q) in sublattice A_l (B_l). Starting from the Schrödinger equation

$$\mathcal{H}|\psi\rangle = E|\psi\rangle,$$

with (3.15) and (3.16), (3.17), following a similar analysis as in monolayer case, we arrive at

$$\hat{\mathcal{H}} \begin{pmatrix} \psi^{A_1} \\ \psi^{B_1} \\ \psi^{A_2} \\ \psi^{B_2} \end{pmatrix} = E \begin{pmatrix} \psi^{A_1} \\ \psi^{B_1} \\ \psi^{A_2} \\ \psi^{B_2} \end{pmatrix}, \quad \hat{\mathcal{H}} = \begin{pmatrix} 0 & -t\phi(\vec{k}) & -\gamma_1 & 0 \\ -t\phi^*(\vec{k}) & 0 & 0 & -\gamma_3\phi^*(\vec{k}) \\ -\gamma_1 & 0 & 0 & -t\phi^*(\vec{k}) \\ 0 & -\gamma_3\phi(\vec{k}) & -t\phi(\vec{k}) & 0 \end{pmatrix}. \quad (3.18)$$

Figure 6: a) Bilayer graphene with upper triangular lattices A_1 (red), B_1 (blue) and lower triangular lattices A_2 (red), B_2 (blue). The hopping parameter between sites A_1 and A_2 is γ_1 and among sites B_1 and B_2 is γ_3 . b) Dispersion relation for bilayer graphene within the low energy approximation.

Let us introduce now a minimal low energy model. In this model, the hopping integral γ_3 is neglected and the only interaction between layers is γ_1 . Then the Hamiltonian $\hat{\mathcal{H}}$ (3.18) becomes

$$\hat{\mathcal{H}} = \begin{pmatrix} 0 & -t\phi(\vec{k}) & -\gamma_1 & 0 \\ -t\phi^*(\vec{k}) & 0 & 0 & 0 \\ -\gamma_1 & 0 & 0 & -t\phi^*(\vec{k}) \\ 0 & 0 & -t\phi(\vec{k}) & 0 \end{pmatrix} \quad (3.19)$$

and the solution to the $\det(\hat{\mathcal{H}} - \mathcal{E}E) = 0$ gives the bilayer graphene dispersion relation

$$E(\vec{k}) = s_1 \left(s_2 \frac{\gamma_1}{2} + \sqrt{\frac{\gamma_1^2}{4} + t^2 |\phi(\vec{k})|^2} \right), \quad s_1, s_2 = \pm, \quad (3.20)$$

where close to the Dirac point $\mathbf{K}$, we write $\vec{k} = \mathbf{K} + \vec{p}$ and have $t\phi(\vec{k}) \approx \frac{3}{2}a_{CC}tp = \hbar v_F p$, with $p = (ip_x - ip_y)$. In the low energy limit ($\hbar v_F < \gamma_1$), $E(\vec{k})$ consists of two parabolas separated by γ_1 .

In bilayer graphene, the application of an external electric field leads to a potential difference between layers ($2V$), which incorporated in the Hamiltonian $\hat{\mathcal{H}}$ (3.19) reads

$$\hat{\mathcal{H}} = \begin{pmatrix} -V & -t\phi(\vec{k}) & -\gamma_1 & 0 \\ -t\phi^*(\vec{k}) & -V & 0 & 0 \\ -\gamma_1 & 0 & V & -t\phi^*(\vec{k}) \\ 0 & 0 & -t\phi(\vec{k}) & V \end{pmatrix}$$

and lead the band gap opening in the vicinity of the $\mathbf{K}$ points. The gap is directly proportional to the applied bias $2V$.

3.3 Quantum dots

There are several types of graphene quantum dots, including [26]

- islands
- field-induced dots.

Graphene islands are defined by the geometry and mechanical cuts of graphene flakes. Field-induced dots are created by the application of electric and magnetic fields. Here we focus on the field-induced dots and explain why it is not possible to confine graphene electrons via electrostatic potential only.

The main problem in graphene confinement is due to Klein-tunneling [13]. Graphene electrons behave like massless particles. When they tunnel high and wide barriers in the normal direction, their transmission probability is close to one. This behaviour is strikingly different than in conventional semiconductors, where electrons with energies lower than the barrier height are almost completely reflected (the probability of transmission decays exponentially as the energy decrease). Klein tunnelling of graphene electrons can be explained through the link between graphene positively and negatively charged states. A sufficiently strong potential, that is repulsive for electrons, is attractive for holes. What happens in graphene is that an electron state outside a potential barrier align with a hole states inside the barrier, leading to a high transmission probability. To suppress that transmission one needs to use additional means, for example apply a high magnetic field.

Figure 7: Schemat of the scattering problem. The nanoribbon is divided into three regions: two semi-infinite leads (in blue) and the scattering region in the middle with an example potential $\mathcal{P}(x, y)$. The incoming waves have amplitudes A_L and A_R and the outgoing ones have B_L and B_R .

4 Transport and scattering in nanoribbons

4.1 The Landauer approach

The Landauer approach is used to describe transport through mesoscopic devices. This formalism allows to express a current in terms of transmission probabilities. In particular, the Landauer formula relates the conductance G (the ease at which the current passes through a device) to the transmission $\mathcal{T}$ [6]

$$G = \frac{2e^2}{h} \mathcal{T}, \quad (4.1)$$

where h is a Planck's constant. The transmission $\mathcal{T}$ can be calculated from the Green's function.

4.2 Scattering in the discrete tight-binding model

Let us assume that the nanoribbon is parallel with the x axis and that its Hamiltonian is within the tight-binding model (2.5).

Consider a scattering problem. The scattering on a potential $\mathcal{P}(x, y)$ takes place in the nanoribbons region $0 \leq x \leq l$, that is connected to the left and to the right to semi-infinite leads (Figure 7). Far from the scattering regions, the Schrödinger equation

$$H\Psi = E\Psi$$

defines the scattering states. The scattering matrix S relates the outgoing amplitudes (B_L, B_R) to the incoming ones (A_L, A_R)

$$\begin{pmatrix} B_L \\ B_R \end{pmatrix} = S \begin{pmatrix} A_L \\ A_R \end{pmatrix},$$

where A_L, A_R, B_L, B_R are all vectors of size n , that is equal to the number of the transmission channels. In particular consider $n = 1$. If an incoming state from the left has amplitude $A_L = 1$, then it is reflected to an outgoing state to the left with coefficient (reflection probability) r and transmitted to the outgoing state to the right with coefficient (transmission probability) t . Similarly, if an incoming state from the right has amplitude $A_R = 1$, then it is reflected to an outgoing state to the left with coefficient r' and transmitted to the outgoing state to the right with coefficient t' . This example explains the nomenclature of the scattering matrix elements as

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}, \quad (4.2)$$

even if in the general case a total incoming state is a linear combination of all the incoming states and matrix S is $2n \times 2n$. Such defined scattering matrix is unitary.

The total transmission and reflection amplitude can be expressed through the elements of the scattering matrix S and the group velocities of the states, namely

$$\mathcal{T} = \sum_{\alpha, \beta} \frac{v_\beta}{v_\alpha} |t_{\beta\alpha}|^2, \quad \mathcal{R} = \sum_{\alpha, \beta} \frac{v_\beta}{v_\alpha} |r_{\beta\alpha}|^2 \quad (4.3)$$

where α and β are transmission channels; $t_{\beta\alpha}, r_{\beta\alpha}$ are elements of matrices $[t]_{\beta\alpha}$ and $[r]_{\beta\alpha}$, define it (4.2), they describe transmission and reflection amplitudes from state α to state β ; v_α, v_β are velocities (defined later in (4.9)). Note that velocities define the direction of the propagation.

The transmission and reflection coefficients can be derived from the fluxes of the quantum mechanical current, what is presented by the end of Sect. 4.2.2.

4.2.1 The Green's function

The Green's function can be defined as the response at any point of the material due to the excitation at any other point of the material. Having

$$[E - H]\Psi = f, \quad (4.4)$$

with Hamiltonian H , energy E (it may be complex), excitation f and the wavefunction Ψ describing the response, the Green's function is defined as a solution to equation

$$[E - H(\vec{x})]G(\vec{x}, \vec{x}', E) = \delta(\vec{x} - \vec{x}'). \quad (4.5)$$

subject to certain boundary conditions. The Green's function is the kernel of the inverse operator $[E - H]^{-1}$ which we will denote as³

$$G(E) = [E - H]^{-1}. \quad (4.6)$$

³We may refer to operator $G(E)$ as a Green's function, what is often done in physics books

Now, due to the linearity of $E - H(\vec{x})$ the solution to equation (4.4) is just $\Psi(\vec{x}) = \sum_{\vec{x}'} G(\vec{x}, \vec{x}', E) f(\vec{x}')$.

The Green's function can be expressed through the eigenfunctions of the operator $E - H$ [7]

$$G(\vec{x}, \vec{x}', E) = \sum_m \frac{\Psi_m(\vec{x}) \Psi_m^*(\vec{x}')}{E - E_m} + \int dc \frac{\Psi_c(\vec{x}) \Psi_c^*(\vec{x}')}{E - E_c}, \quad (4.7)$$

where the summation is over the discrete spectrum and the integration over the continuous one.

When the spectrum of the operator is continuous, as it is for graphene nanoribbons, $G(\vec{x}, \vec{x}', E)$ is not well defined for E in the continuous spectrum, however one can define $G(\vec{x}, \vec{x}', E)$ by a limiting procedure. For graphene nanoribbons the eigenfunctions associated with the continuous spectrum are propagating states (or extended) and their Bloch form is

$$\Psi_\alpha(x, y) = e^{ik_\alpha x} \chi_\alpha(y),$$

where α is a transverse mode and $\chi_\alpha(y)$ is a transverse mode wavefunction. One can define uniquely the Green's function on the continuous spectrum by its behaviour at infinities introducing the retarded Green's function

$$G(\vec{x}, \vec{x}', E) = \lim_{\eta \rightarrow 0^+} G(\vec{x}, \vec{x}', E + i\eta).$$

Thanks to this definition and (4.7), the Green's function of a pristine nanoribbon can be expressed as

$$G^0(x, y; x', y'; E) = \begin{cases} -\sum_\alpha \frac{i}{v_\alpha} \chi_\alpha(y) \chi_\alpha^*(y') e^{ik_\alpha(x-x')}, & x > x' \\ -\sum_\alpha \frac{i}{v_\alpha} \chi_\alpha^*(y) \chi_\alpha(y') e^{-ik_\alpha(x-x')}, & x < x' \end{cases}, \quad (4.8)$$

where the superscript '0' indicates the pristine nanoribbon and

$$\sum_y \chi_\beta^*(y) \chi_\alpha(y) = \delta_{\beta, \alpha}.$$

Let us now consider scattering on a potential $\mathcal{P}(x, y)$. The potential $\mathcal{P}(x, y)$ can be included in the Hamiltonian H and the total Green's function can be obtained through the inverse operator (considered later in this Section) or the Dyson equation (considered in Sect. 4.2.2). The transmission amplitudes between modes α and β are related to the total Green's function through the Fisher-Lee formula [6]

$$t_{\beta\alpha} = i\sqrt{v_\alpha v_\beta} \sum_{y, y'} \chi_\beta^*(y) e^{-ik_\beta x} G(x, y; x', y'; E) \chi_\alpha(y') e^{ik_\alpha x'}$$

with x' and x both taken outside the scattering region (in particular to the left and to the right of it), and velocities defined as

$$v_\alpha = \frac{\partial E}{\partial k_\alpha}. \quad (4.9)$$

4.2.2 The recursive Green's function technique

The Green's function (4.8) is defined for a pristine nanoribbon. It is possible to calculate the Green's function for nanoribbons with very simple potentials, like a defect in one point of the lattice. The Green's function of the structures with more complicated scatterers can be obtained numerically through the matrix inversion (4.6). However, it is very inefficient to inverse a large matrix. To make calculations more efficient, the recursive Green's function technique was introduced [25, 28, 29, 11]. In this method, a nanoribbon is divided into three regions: left lead, a region with a scattering potential and right lead. Now, the intermediate scattering region is sliced and an inverse (4.6) is calculated separately for each slice. The total Green's function is obtained from the recursive coupling of the slices and finally by the connection with the surface Green's function of the two leads.

The recursive Green function technique is used in numerical simulations. Let present six instruments and meta results which are important for the computation of the transmission and reflection coefficients in graphene nanoribbons. For the purpose of this analysis, let us assume that the nanoribbons tight-binding Hamiltonian is expressed as

$$H = \sum_{i,j} \mathcal{P}_{ij} a_{ij}^\dagger a_{ij} - t \sum_{i,j,\Delta} (a_{ij}^\dagger a_{ij+\Delta} + a_{ij+\Delta}^\dagger a_{ij}), \quad (4.10)$$

with creation/annihilation operators $a_{ij}^\dagger/a_{ij}$, where this time i denotes the slice number and j the orbitals position within the slice, Δ runs over the nearest-neighbours of orbital (i, j) and $\mathcal{P}_{ij}$ is an onsite potential. Similarly the wave function is

$$|\Psi\rangle = \sum_{i,j} \psi_{ij} a_{ij}^\dagger |0\rangle. \quad (4.11)$$

Now, we are ready to sketch the technique.

1. The unit cell is defined (Figure 8) as a sum of M slices ($1 \leq m \leq M$, $M = 2$ for zigzag and $M = 4$ for armchair) with a Green's function of a single slice calculated via matrix inversion. The total scattering region is a sum of unit cells with onsite potentials or it is just one unit cell, when a pristine structure is assumed.

2. The coupling between a single strip Green's function is defined through the Dyson Equation. Here we present a simple derivation of the Dyson equation.

Let us consider Hamiltonians of two strips (H_1^0, H_2^0) and the interaction V between them (nearest-neighbour hopping). The total Hamiltonian of the system is

$$H = H^0 + V, \quad \text{with} \quad H^0 = H_1^0 + H_2^0.$$

The inverse operator is

$$G = [E - H^0 - V]^{-1} = [(E - H^0)(I - G^0 V)]^{-1} = (I - G^0 V)^{-1} G^0$$

and multiplying from the left by $(I - G^0 V)$, we arrive at the Dyson equation

$$G = G^0 + G^0 V G.$$

Figure 8: Model of graphene nanoribbon (zigzag) with two semi-infinite leads (blue) and the scattering region in between. A unit cell in the scattering region is indicated in the yellow rectangle. The scattering region can be divided into slices (purple). Armchair nanoribbon is modelled in a very similar way, however with four slices per unit cell.

The operator G that is associated with the Green's function can be viewed as a propagator that specifies the probability amplitude for a particle to move from one place to another. That is why the Dyson equation can be written as an infinite sum ($G = \sum_{n=1}^{\infty} G_0 (V G_0)^n$) and interpreted as a sum of all possible particle paths (Feynman paths) with no scattering by V , with one scattering by V , two (passage, scattering, reflection, scattering, passage) and so on.

Now, having a Green function of two strips, we can couple it to the third strip and so on. In this way, we omit the inversion of a huge matrix of square size the number of all atoms; however we still need to obtain G^0 , again by a matrix inversion, but this time with a matrix size being the square of the number of atoms squared in the unit cell!

3. The Bloch states (2.3) are used to formulate an eigenvalue problem and find k -values describing the propagating modes. Here we present how this is done. The total Hamiltonian (4.10) and total wavefunction of the system (4.11) can be simply divided into the following parts

$$H = H_{\text{scatt}} + H_{\text{leads}} + V_{\text{sl}}, \quad |\Psi\rangle = |\Psi_{\text{scatt}}\rangle + |\Psi_{\text{leads}}\rangle$$

where H_{scatt} , H_{leads} describes the hopping in the scattering region and leads respectively and V_{sl} is the interaction between them. Now, let us use the Schrödinger equation $H|\Psi\rangle = E|\Psi\rangle$ to get a relation for the sites of the scattering region. In that case note that

$$\langle 0 | a_{ij} V_{\text{sl}} | \Psi_{\text{scatt}} \rangle = \langle 0 | a_{ij} V_{\text{sl}} | \Psi_{\text{scatt}} \rangle = \langle 0 | a_{ij} V_{\text{sl}} | \Psi_{\text{scatt}} \rangle = 0,$$

with (i, j) in the scattering region, moreover

$$H_{\text{scatt}}|\Psi_{\text{leads}}\rangle = 0, \quad H_{\text{leads}}|\Psi_{\text{scatt}}\rangle = 0,$$

what leads us to the final form of the wave function in the scattering region

$$|\Psi_{\text{scatt}}\rangle = G_{\text{scatt}}V_{\text{sl}}|\Psi_{\text{leads}}\rangle, \quad (4.12)$$

where $G_{\text{scatt}} = (E - H_{\text{scatt}})^{-1}$ and $V_{\text{sl}}|\Psi_{\text{leads}}\rangle$ is considered to be a source (excitation). To make use of the last equation, it is necessary to assume the Bloch form of the states

$$\psi_{m+M} = e^{ikx_M}\psi_m, \quad (4.13)$$

with

$$\psi_m = \begin{pmatrix} \psi_{m1} \\ \vdots \\ \psi_{mN} \end{pmatrix} \quad (4.14)$$

being a vector with wavefunction in one of the slices with $1 \leq m \leq M$ or $m = 0$ and $m = M + 1$ when it belongs to the slice on the edge of the left/right lead (Figure 8), x_M is a coordinate of M -th slice. Then calculating the matrix elements $\psi_{1j} = \langle 0|a_{1j}|\Psi_{\text{scatt}}\rangle$ and $\psi_{Mj} = \langle 0|a_{Mj}|\Psi_{\text{scatt}}\rangle$ in (4.12) and defining

$$(G_{\text{scatt}}^{ii'})_{jj'} = \langle 0|a_{i'j'}G_{\text{scatt}}a_{ij}|0\rangle, \quad (V_{ii'})_{jj'} = \langle 0|a_{i'j'}V a_{ij}|0\rangle$$

allows us to set up an eigenvalue problem that reads

$$T_1^{-1}T_2 \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix} = e^{ikx_M} \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix},$$

with ψ_0 and ψ_1 defined as in (4.14) and

$$T_1 = \begin{pmatrix} -G_{\text{scatt}}^{1,M}V_{1,0}^t & 0 \\ -G_{\text{scatt}}^{M,M}V_{1,0}^t & \mathcal{I} \end{pmatrix}, \quad T_2 = \begin{pmatrix} -\mathcal{I} & G_{\text{scatt}}^{1,1}V_{1,0} \\ 0 & G_{\text{scatt}}^{M,1}V_{1,0} \end{pmatrix}$$

where we used $V_{M+1,M} = V_{0,1}$ and $V_{0,1} = V_{1,0}^t$. The eigenvalues of this problem give k vectors. Those for the propagating modes (with real value of k) are denoted k^α with a mode number $1 \leq \alpha \leq N$.

4. The direction of the propagation of a mode is defined through the velocity.

The group velocity is defined in (4.9), however let's us derive a more explicit expression. First of all, the wavefunction of the Bloch state in α mode can be written as

$$|\psi\rangle = \sum_{i=1}^M |\psi_i\rangle \quad (4.15)$$

where $|\psi_i\rangle$ is the wavefunction of the i -th slice and M is the number of slices, using the Bloch form of the waves

$$|\psi_i\rangle = e^{ik_\alpha x_i} |\phi_i\rangle, \quad (4.16)$$

and

$$\phi_i = \begin{pmatrix} \phi_{i1} \\ \dots \\ \phi_{iN} \end{pmatrix} \quad (4.17)$$

with $\phi_{ij} = \langle 0 | a_{ij} | \phi \rangle$, we can express the energy as

$$E = \frac{1}{M} \sum_{i=1}^M \frac{\langle \psi_i | H | \psi \rangle}{|\phi_i|^2}, \quad (4.18)$$

with the Hamiltonian H of the scattering region

$$H = \sum_{i=1}^M H_i^0 + \sum_{i=0}^M V_{i,i+1}, \quad (4.19)$$

where H_i^0 is a Hamiltonian of a single slice i and $V_{i,i+1}$ is the hopping matrix between slices i and $i+1$. Then the velocity becomes

$$\begin{aligned} v &= \frac{\partial E}{\partial k} = \frac{1}{M} \sum_{i=1}^M \frac{\partial}{\partial k} \frac{\langle \psi_i | H | \psi \rangle}{|\phi_i|^2} \\ &= \frac{-i}{M} \sum_{i=1}^M \frac{\phi_i^{*T}}{|\phi_i|^2} \left((x_i - x_{i-1}) V_{i,i-1} \phi_{i-1} e^{-ik_a(x_i - x_{i-1})} - (x_{i+1} - x_i) V_{i,i+1} \phi_{i+1} e^{-ik_a(x_{i+1} - x_i)} \right). \end{aligned} \quad (4.20)$$

5. The surface Green's function

One can imagine that it could be possible to proceed with coupling the single slices until the infinity, that is $M \rightarrow \infty$. This is not the case as the propagating waves are defined in the infinite region only, while in the finite region the wavefunctions have the form of standing waves. That is why we need to calculate the surface Green's functions (left and right) that will describe the effect of the leads. For graphene nanoribbons, one can derive the analytical expression of those functions. To get the expression for the right surface Green's function, let us consider a semi-infinite nanoribbon, separated into two regions with $1 \leq i \leq M$ and with $M+1 \leq i \leq \infty$. Then, the right surface Green function is defined as $\Gamma_R := G_{11}^0$ with $G_{ii'}^0$ being a matrix with elements $\langle 0 | a_{i'j'} G^0 a_{ij} | 0 \rangle$ for $j, j' = 1, \dots, N$ of Green function G^0 of one of the two considered regions. Note that $G_{00}^0 = G_{M+1, M+1}^0$ as the regions $0 \leq i \leq \infty$ and $M+1 \leq i \leq \infty$ are identical from the physical point of view. The definition of the Green's function says

$$|\Psi\rangle = G|s\rangle, \quad (4.21)$$

with source (excitation) $|s\rangle$, the Green's function of the semi-infinite nanoribbon G and response $|\Psi\rangle$. In particular assuming the source at the boundary slice $i = 0$, we have $|s\rangle = \sum_{j=1}^N \psi_{0j} a_{0j}^\dagger |0\rangle$ and multiplying (4.21) by $\langle 0 | a_{M+1,j}$ from the left we get the response at slice $M+1$ given by

$$\psi_{M+1} = G_{M+1,0} \psi_0. \quad (4.22)$$

Let us apply the Dyson relation between slices M and $M+1$

$$G_{M+1,0} = G_{M+1,0}^0 + G_{M+1,M+1}^0 V_{M+1,M} G_{M0} = \Gamma_R V_{1,0} G_{M0}, \quad (4.23)$$

as $G_{M+1,0}^0 = 0$ as $G_{i,j}^0 = 0$ when then slices i and j belong to different regions. Now using (4.23) and (4.22), we get

$$\psi_{M+1} = \Gamma_R V_{1,0} G_{M0} \psi_0 = \Gamma_R V_{1,0} \psi_M$$

and recalling the Bloch form of states with k_α , we can write

$$\psi_1^\alpha = \Gamma_R V_{1,0} \psi_0^\alpha$$

and finally

$$\Gamma_R V_{1,0} = \Psi_1 (\Psi_0)^{-1},$$

with $\Psi_i = (\psi_i^1, \dots, \psi_i^N)$, $i = 1, 2$, where the lower index indicates a slice number and the upper one the mode number $(k_1, \dots, k_N)$. In our case (no magnetic field), $\Gamma_R = \Gamma_L$ holds.

6. Transmission and reflection coefficients can be expressed through the Green's function. Let us consider an incoming state $|\psi_{\text{inc}}^\alpha\rangle$ from the left lead, that scatters in a scattering region $[0, L]$ into a transmitted state $|\psi_{\text{trans}}^\alpha\rangle$ (in the right lead) and reflected state $|\psi_{\text{refl}}^\alpha\rangle$ (in the left lead) with

$$|\psi_{\text{inc}}^\alpha\rangle = \sum_{l \leq 0} e^{ik_\alpha^+ x_l} \sum_{j=1}^N \psi_{lj}^\alpha a_{l,j}^\dagger |0\rangle, \quad (4.24)$$

$$|\psi_{\text{trans}}^\alpha\rangle = \sum_{l \geq L} \sum_{\beta} t_{\beta\alpha} e^{ik_\beta^+ (x_l - x_M)} \sum_{j=1}^N \psi_{lj}^\beta a_{l,j}^\dagger |0\rangle, \quad (4.25)$$

$$|\psi_{\text{refl}}^\alpha\rangle = \sum_{l \leq 0} \sum_{\beta} r_{\beta\alpha} e^{ik_\beta^- x_l} \sum_{j=1}^N \psi_{lj}^\beta a_{l,j}^\dagger |0\rangle, \quad (4.26)$$

where the values k_α have superscript '+' for states propagating to the right and '-' for those propagating to the left. The amplitudes $t_{\beta\alpha}$ and $r_{\beta\alpha}$ can be obtained from the Green's functions through the following formulas

$$\Psi_1 t = -G^{L,0} (V_{0,1} \Psi_1 K - \Gamma_L^{-1} \Psi_0),$$

$$\Psi_0 r = -G^{0,0} (V_{0,1} \Psi_1 K - \Gamma_L^{-1} \Psi_0) - \Psi_0,$$

where elements $t_{\beta\alpha}$ composite matrix t and $r_{\beta\alpha}$ composite matrix r , then K is a diagonal matrix with elements $(K)_{\alpha,\alpha} = \exp(ik_\alpha^+ x_1)$.

Finally, let us derive the formulas for the total transmission and reflection (4.3).

The total transmission and reflection coefficients are defined through the transfer of quantum mechanical current in x direction (parallel with the nanoribbon), which for Hamiltonian (4.19) and a Bloch state in α mode (4.2.2) is

$$j = \frac{e}{LW} \frac{-i}{M} \sum_1^M \frac{\phi_i^{*T}}{|\phi_i|^2} \left((x_i - x_{i-1}) V_{i,i-1} \phi_{i-1} e^{-ik_\alpha(x_i - x_{i-1})} - (x_{i+1} - x_i) V_{i,i+1} \phi_{i+1} e^{-ik_\alpha(x_{i+1} - x_i)} \right), \quad (4.27)$$

where e is the unit charge, L is the nanoribbon width and W is the width of a single slice (Figure 8).

Now the transmission and reflection coefficients are defined as the ratios of current fluxes

$$\mathcal{T} = \sum_{\alpha,\beta} \frac{j_{\text{trans}}^{\beta\alpha}}{j_{\text{inc}}^{\alpha}} = \sum_{\alpha,\beta} \frac{v_\beta}{v_\alpha} |t_{\beta\alpha}|^2, \quad \mathcal{R} = \sum_{\alpha,\beta} \frac{j_{\text{refl}}^{\beta\alpha}}{j_{\text{inc}}^{\alpha}} = \sum_{\alpha,\beta} \frac{v_\beta}{v_\alpha} |r_{\beta\alpha}|^2 \quad (4.28)$$

where j_{inc}^{α} , $j_{\text{trans}}^{\beta\alpha}$, $j_{\text{refl}}^{\beta\alpha}$ are incoming, transmitted and reflected fluxes from channel α to channel β and they are calculated from the expression for incoming, transmitted and reflected states (4.24), (4.25), (4.26), which are sums of Bloch waves with certain coefficients. The second equalities in (4.28) for current fluxes come from the comparison of expression for current (4.27) with the expression for velocity (4.20). Now the conductance can be calculated from the Landauer formula (4.1).

5 Electron-electron interactions

In the previous sections, we considered the Schrödinger equation for a single electron described by a wavefunction of its position $\vec{x}$. In reality, the behaviour of one charged particle depends on all the other charged particles present in the material, and there are many of them. In this section we formulate a many body problem. This problem is analytically solvable for two particles only but it can be numerically solved under certain approximations.

5.1 The many body problem

The many-body Hamiltonian is [17]

$$H = - \sum_{j=1}^{N_e} \frac{\hbar^2 \nabla_j^2}{2m_e} + \frac{1}{8\pi\epsilon\epsilon_0} \sum_{\substack{j,i \\ j \neq i}}^{N_e} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} - \sum_{I=1}^{N_n} \frac{\hbar^2 \nabla_I^2}{2M_I} \quad (5.1)$$

$$+ \frac{1}{8\pi\epsilon\epsilon_0} \sum_{I \neq J}^{N_n} \frac{Z_I Z_J e^2}{|\vec{R}_I - \vec{R}_J|} - \frac{1}{8\pi\epsilon\epsilon_0} \sum_{j=1}^{N_e} \sum_{I=1}^{N_n} \frac{Z_I e^2}{|\vec{r}_j - \vec{R}_I|} \quad (5.2)$$

where the electrons are denoted by the lower case subscripts with position $\vec{r}_i$ and mass m_e , and nuclei by upper case subscripts with position $\vec{R}_I$, charge Z_I and mass M_I . The number of electrons/nuclei is N_e , respectively N_n and ϵ_0 , ϵ denote vacuum permittivity and permittivity (the effect of the material type on the Coulomb interaction within it). The first two terms in Hamiltonian (5.1) composite the electronic Hamiltonian: the kinetic energy of electrons and interaction between them; the following two terms composite the nuclear Hamiltonian: the kinetic energy of nuclei and their interaction; and the final term is the attraction between nuclei and electrons. Now, the Schrödinger equation for a many body system is

$$H\Psi(\{\vec{r}_i\}; \{\vec{R}_I\}) = E\Psi(\{\vec{r}_i\}; \{\vec{R}_I\}),$$

with the many-body wavefunction

$$\Psi(\{\vec{r}_i\}, \{\vec{R}_I\}) \equiv \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{N_e}; \vec{R}_1, \vec{R}_2, \dots, \vec{R}_{N_n}).$$

One term in Hamiltonian (5.1) can be regarded as small, namely the kinetic energy of nuclei, due to their relatively big mass M_I . This term is ignored in the Born-Oppenheimer approximation. It follows that the positions of nuclei become parameters and the interaction between nuclei and electrons can be included in the external potential; moreover the wavefunction is $\Psi = \Psi(\{\vec{r}_i\})$.

5.2 The independent electron approximation

The total Hamiltonian that we do consider now is [17]

$$H = - \sum_{j=1}^{N_e} \frac{\hbar^2 \nabla_j^2}{2m_e} + \frac{1}{8\pi\epsilon\epsilon_0} \sum_{\substack{j,i \\ j \neq i}}^{N_e} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} + \sum_{i=1}^{N_e} V(\vec{r}_i), \quad (5.3)$$

where $V(\vec{r}_i)$ is the external potential (that includes all the effects of nuclei). Next step is to treat electrons as independent particles, moving in the field created by the remaining electrons. There are two types of independent electron approximations

- Hartree
- Hartree-Fock.

The difference between them is the consideration of the exchange interaction due to the Pauli principle, neglected in the Hartree approximation and included in the Hartree-Fock.

In the Hartree method the total wave function is expressed as a product of single particle wave functions

$$\Psi(\{\vec{r}_i\}) = \prod_{i=1}^{N_e} \psi_i(\vec{r}_i). \quad (5.4)$$

Using the variational principle (minimising the expectation value $\langle \Psi | H | \Psi \rangle$ of the Hamiltonian H (5.3)), we arrive at a system of N_e coupled equations for N_e single particle wavefunctions

$$\left[-\frac{\hbar^2 \nabla^2}{2m_e} + \frac{e^2}{4\pi\epsilon\epsilon_0} \sum_{j \neq i}^{N_e} \int \frac{|\psi_j(\vec{r}')|^2}{|\vec{r} - \vec{r}'|} d\vec{r}' + V(\vec{r}) \right] \psi_i(\vec{r}) = E_i \psi_i(\vec{r}), \quad (5.5)$$

where the second term on the left-hand side is called Hartree term.

The second method, Hartree-Fock, assumes that the total wave function is the Slater determinant of N_e single particle wavefunctions

$$\Psi(\{\vec{r}_i\}) = \frac{1}{\sqrt{N_e!}} \begin{vmatrix} \psi_1(\vec{r}_1) & \dots & \psi_{N_e}(\vec{r}_1) \\ \vdots & \ddots & \vdots \\ \psi_1(\vec{r}_{N_e}) & \dots & \psi_{N_e}(\vec{r}_{N_e}) \end{vmatrix},$$

where the single particle wave functions $\psi(\vec{r}_i)$ may depend on the spin. This construction preserves the antisymmetry of the total wave function due to the Pauli principle (antisymmetry due to the switch between two electrons). Now, through the variational principle, the Schrödinger equation becomes

$$\begin{aligned} \left[-\frac{\hbar^2 \nabla^2}{2m_e} + \frac{e^2}{4\pi\epsilon\epsilon_0} \sum_{j \neq i}^{N_e} \int \frac{|\psi_j(\vec{r}')|^2}{|\vec{r} - \vec{r}'|} d\vec{r}' + V(\vec{r}) \right] \psi_i(\vec{r}), \\ - \frac{e^2}{4\pi\epsilon\epsilon_0} \sum_{j \neq i}^{N_e} \int \frac{\psi_j^*(\vec{r}') \psi_i(\vec{r}')}{|\vec{r} - \vec{r}'|} d\vec{r}' \psi_j(\vec{r}) = E_i \psi_i(\vec{r}). \end{aligned} \quad (5.6)$$

It is important to note the non-linearity (non-locality) of the additional term (with respect to equation (5.5)). This term is an exchange-correlation term and it is a consequence of the Pauli exclusion principle.

5.3 The density functional theory

Still, the system of equations (5.5) or (5.6) is huge. In this section, we consider the next approximation namely substitution of the quantum mechanical wavefunctions in (5.5), (5.6) by the classical electrons density. There are two possible approaches, the Thomas-Fermi theory (TF) that uses electron density, and Density Functional Theory (DFT), that uses both electron density and single electron wavefunctions. TF is a precursor of DFT; however here we begin by presenting the more general DFT for motivation (Theorems 1 and 2) and make a few simplifications to obtain TF.

DFT assumes that the properties of the system of N_e electrons can be determined through the functionals of the electrons density, defined as

$$n(\vec{r}) = e \int |\Psi(\vec{r}, \vec{r}_2, \dots, \vec{r}_{N_e})|^2 d\vec{r}_2 \dots d\vec{r}_{N_e}. \quad (5.7)$$

This assumption is backed by two Hohenberg-Kohn (KH) theorems, which are core of DFT and read [17, 12, 14]

Theorem 1. For any system of interacting particles in external potential $V_{\text{ext}}(\vec{r})$, the potential $V_{\text{ext}}(\vec{r})$ is determined uniquely, by the ground state particle density $n_0(\vec{r})$.

and

Theorem 2. A universal functional for the energy $E[n]$ in terms of electrons density $n(\vec{r})$ can be defined, valid for any external potential $V_{\text{ext}}(\vec{r})$. For any particular $V_{\text{ext}}(\vec{r})$, the exact ground state energy of the system is the global minimum value of this functional, and the density that minimizes the functional is the ground state density.

Those theorems prove that in principle the ground state density determines everything. Now, the Kohn-Sham (KS) ansatz, used to find the the ground state density, assumes that the ground state density of the many body problem (with Hamiltonian (5.3)) is equal to a chosen ground state density of the auxiliary problem of non interacting particles moving in an effective potential (V_{eff}). Consequently by solving the auxiliary problem, we obtain the solution to the original one according to the KH theorems.

The ground state solution to the KS auxiliary problem can be found by minimising the following functional with respect to $n(\vec{r})$

$$E[n(\vec{r})] = T[n(\vec{r})] + \int V_{\text{eff}}(\vec{r}) n(\vec{r}) d\vec{r}, \quad (5.8)$$

with electrons density

$$n(\vec{r}) = e \sum_i^{N_e} |\psi_i(\vec{r})|^2$$

effective potential

$$V_{\text{eff}}(\vec{r}) = V_{\text{ext}}(\vec{r}) + V_{\text{Hartree}}(\vec{r}) + V_{\text{xc}}(\vec{r}), \quad (5.9)$$

Hartree term

$$V_{\text{Hartree}}(\vec{r}) = \frac{e^2}{4\pi\epsilon\epsilon_0} \int \frac{n(\vec{r}')}{|\vec{r} - \vec{r}'|} d\vec{r}',$$

and where $V_{\text{xc}}(\vec{r})$ accounts for all the quantum mechanical effects coming from the exchange term in the Hartree-Fock approximation (5.6). The kinetic energy term is calculated as

$$T[n(\vec{r})] = \sum_{i=1}^{N_e} \int \psi_i^* \left(-\frac{\hbar^2 \nabla^2}{2m_e} \right) \psi_i d\vec{r},$$

with the wavefunctions being the solutions to the Schrödinger equation

$$\left[-\frac{\hbar^2 \nabla^2}{2} + V_{\text{eff}} \right] \psi_j(\vec{r}) = E_j \psi_j(\vec{r}). \quad (5.10)$$

Equations (5.9) and (5.10) can be solved in the self consistent way

$$V_{\text{eff}} \rightarrow \psi_i \rightarrow \psi_0 \rightarrow n_0 \rightarrow V_{\text{eff}},$$

where ψ_0 and n_0 denote the wavefunction and electrons density of the ground state.

5.4 The Thomas Fermi approximation

There are a few assumptions in the TF approximation that make it simpler than the DFT approximation. First of all the TF approximation is based on Hartree interaction and so the exchange term that accounts for the quantum mechanical interaction is neglected and the effective potential in (5.9) becomes

$$V_{\text{eff}}(\vec{r}) = V_{\text{ext}}(\vec{r}) + V_{\text{Hartree}}(\vec{r}). \quad (5.11)$$

When atoms have discrete positions (j), one can account for self-interaction in the Hartree term writing [8, 27]

$$V_{\text{Hartree}}(\vec{r}_j) = \frac{e^2}{4\pi\epsilon\epsilon_0} \sum_{\vec{r}_i \neq \vec{r}_j} \frac{n(\vec{r}_i)}{|\vec{r}_j - \vec{r}_i|}.$$

The crucial assumption of the TF approximation is that the kinetic energy is a local functional of electrons density

$$T[n(\vec{r})] = \int t[n(\vec{r})] n(\vec{r}) d\vec{r}.$$

Thanks to this assumption, the Schrödinger equations (5.10) needed to calculate the kinetic energy term in DFT, does not need to be solved. The second very important assumption of the TF theory is that the potential V_{ext} varies slowly with $\vec{r}$. Within those

postulates, we can minimize (5.8) under the assumption of a constant number of particles $\int n(\vec{r}) d\vec{r} = N_e$ and arrive at

$$t[n(\vec{r})] + V_{\text{eff}} = \mu, \quad (5.12)$$

where $\mu = eV_g$ is the chemical potential of the system and V_g is the gate voltage. The electrons density from the last equation can be resolved to [24, 15]

$$n(\vec{r}) = \int \rho[E - V_{\text{eff}}(\vec{r})] f_{\text{FD}}(E, \mu) dE, \quad (5.13)$$

where ρ is the density of states, describing the number of energy states available in the energy interval; f_{FD} is the Fermi-Dirac distribution function that gives the probability occupancy for an electrons level; in particular at zero temperature $T = 0$, $f_{\text{FD}} = 0$ for $E < \mu$ and $f_{\text{FD}} = 1$ for $E > \mu$.

Solving equations (5.11) and (5.13) self consistently with a small damping factor δ

$$V_{\text{eff}}^{i+1}(\vec{r}) = \delta V_{\text{eff}}^i(\vec{r}) + (1 - \delta) V_{\text{eff}}^{i-1}(\vec{r}),$$

where $i > 2$ is the iteration number, we find the screened potential $V_{\text{eff}}(\vec{r})$.

The TF method requires less computational effort than the DFT method as it doesn't require the calculation of the wavefunctions (5.10). Even though this method does neglect the quantum mechanical effects due to electrons exchange (5.6), it gives good qualitative results. As in article V our main interest is the qualitative effect of electrons screening, we incorporate Thomas-Fermi approximation.

6 Summary of the papers

6.1 Paper I

In paper I, we study electronic transport in graphene monolayer and bilayer nanoribbons with short-range defects. Using the tight-binding model and the Green's function (4.2.1), we analytically calculate the transmission for nanoribbons with a single defect. For many defects, we perform simulations based on the Recursive Green's function technique (4.2.2). Our most important finding is that the transmission is strikingly influenced by the nanoribbons edge type. Zigzag nanoribbons are practically not affected by small concentrations of short range defects placed close to the edges; differently such defects decrease the transmission probability in armchair nanoribbons significantly. When the defect concentration increases, the edges are basically damaged and so the transmission in zigzag and armchair nanoribbons evens out. We connect this behaviour with the effective boundary condition, that does not couple valleys in zigzag nanoribbons, thus hindering scattering.

Our second finding is the presence of Fano resonances. In zigzag nanoribbons a single defect placed close to the edge causes a complete transmission block for a tiny range of energies close to the transition between single and three mode regimes. For armchair nanoribbons, a single defect close to the edge shows a Fano resonance with a wide dip that affects a big range of energies. We attribute the appearance of the resonances to the coupling between a dislocalised state of the nanoribbon and the quasibound state of the defect. Weak coupling in zigzag nanoribbons leads to narrow dips; differently strong coupling in the armchair nanoribbons leads to resonances with wide dips.

6.2 Paper II

In this paper we study the effect of electron-electron interaction in graphene quantum dots defined by an external electrostatic potential and a high magnetic field. The interactions are treated on the semi-classical level in the Thomas-Fermi approximation. Under the assumption of a high magnetic field, the screened potential is calculated in the self-consistent way. The screened potential shows steps/slopes in its profile, that correspond to slopes/steps in the electrons density and so are identified as incompressible/compressible strips. To calculate the energy spectrum of the quantum dot, we insert this potential to the Dirac equation in a high magnetic field and solve it numerically using the finite difference method. The final spectrum of electrons energies as a function of the magnetic field shows energy plateaus.

6.3 Papers III and IV

In Paper III and IV, we consider scattering in zigzag graphene nanoribbons with a ultra-low, long-range potential. Within the continuous Dirac model, we analyse the associated

boundary value problem

$$(\mathcal{D} + \delta \mathcal{P}) \begin{pmatrix} u' \\ v' \end{pmatrix} = \omega \begin{pmatrix} u' \\ v' \end{pmatrix} \quad (6.1)$$

with $\mathcal{D} = \frac{D}{\gamma}$ from (3.2), the boundary conditions (3.1), the scaled energy ω and a small parameter δ , which turns out to be non-elliptic. It follows that the properties of the problem, including the uniqueness of the solution, have to be carefully proved. We set up the scattering problem in the analogous way as in the discrete case (Sect. 4.2); however the description is more mathematically complete for the sake of the research goal. Due to the boundary conditions, the scattering in zigzag nanoribbon on the long-range potential is restricted to one valley. The spectrum of the problem (6.1), (3.1) is continuous and covers the whole real line and the number of propagating states that take part in the scattering depends on the spectrum multiplicity. We identify the energy thresholds, where the multiplicity of the spectrum changes, with the maxima in zigzag dispersion relation (3.7). To find a trapped mode, that is a vector eigenfunction (from L_2 space) with eigenvalue embedded in the continuous spectrum, we artificially extend the scattering problem and include two waves of small exponential growth. In this way, all the information about the scattering process is contained in the augmented scattering matrix. Through the scattering, the non-decaying part of the extended states can be removed. Matching the extended states at infinities, we arrive at the necessary and sufficient condition on the augmented scattering matrix for the existence of the trapped mode. Tuning small parameters of the ultra-low potential, we show that trapped modes exist for energies close and less than a threshold. We also prove that there are no trapped modes with energies slightly bigger or far from the thresholds, provided the potential is sufficiently small.

In Paper III, we present a sketch (a simplified case) of article III, with extended states introduced only in half strip and a different approach for matching than in article IV.

6.4 Paper V

In Paper V, we consider scattering in armchair graphene nanoribbons with a ultra-low, long-range potential. As the associated boundary value problem within the continuous Dirac model

$$(\mathcal{D} + \delta \mathcal{P}) \begin{pmatrix} u \\ v \\ u' \\ v' \end{pmatrix} = \omega \begin{pmatrix} u \\ v \\ u' \\ v' \end{pmatrix} \quad (6.2)$$

with $\mathcal{D} = \frac{D}{\gamma}$ from (2.23), the boundary conditions (3.8), (3.9), the scaled energy ω and a small parameter δ . In contrary to zigzag nanoribbon case, the boundary value problem for armchair nanoribbon is elliptic. Electrons in armchair nanoribbons take part in both types of scattering (inter and intra valley) and a complete problem has to be considered. The spectrum of the problem is continuous and in case of non-metallic ribbons, on which we focus, covers the whole real line without an interval centered at zero. We identify the energy thresholds, where the multiplicity of the spectrum changes. The

value of the first threshold gives the ends of the interval excluded from the continuous spectrum. To find a trapped mode, we artificially extend the scattering problem and include two waves of small exponential growth. Similarly as for zigzag nanoribbons, we base our approach on the augmented scattering matrix, perform asymptotic analysis and give the condition for the existence of the trapped mode. Using this condition and tuning small parameters, we construct a potential that produces a trapped mode with energy slightly less than a threshold. We also prove that there are no trapped modes with energies slightly bigger or far from the thresholds, provided the potential is sufficiently small.

6.5 Paper VI

In paper VI, we give the error estimates between an eigenvalue of a linear differential operator and the numerically computed approximate eigenvalue of the discretized approximation of the operator. First, we prove that the error estimate for the eigenvalue can be obtained from the residual of the approximate eigenpair. Then using a couple of examples, we calculate the residual analytically, applying the differential operator to an approximate eigenfunction interpolated by splines. In particular, we calculate errors for the energy levels in graphene quantum dots considered in paper II.

References

- [1] D.S.L. Abergel, V. Apalkov, J. Berashevich, K. Ziegler and Tapash Chakraborty, *Properties of graphene: a theoretical perspective*, Adv. Phys., 59 (4), 261–482 (2010).
- [2] T. Ando, T. Nakanishi, *Impurity Scattering in Carbon Nanotubes - Absence of Back Scattering*, J. Phys. Soc. Jpn. **67**, 1704-1713 (1998)
- [3] N. W. Ashcroft, N. D. Mermin, *Solid State Physics*, Holt, Rinehart and Winston, New York (1976).
- [4] L. Brey, H. A. Fertig, *Electronic states of graphene nanoribbons studied with the Dirac equation*, Phys. Rev. **B 73**, 235411 (2006).
- [5] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, A. K. Geim, *The electronic properties of graphene*, Rev. Mod. Phys. **81**, 109 (2009).
- [6] S. Datta, *Electronic Transport in Mesoscopic Systems*, Cambridge University Press, Cambridge (1997).
- [7] E. N. Economou, *Green's Functions in Quantum Physics*, Springer, Heidelberg (2006).
- [8] J. Fernández-Rossier, J. J. Palacios, L. Brey, *Electronic structure of gated graphene and graphene ribbons*, Phys. Rev. **B 75**, 205441 (2007).
- [9] A. K. Geim, K. S. Novoselov, *The rise of graphene*, Nat. Mat, **6**, 183 (2007).
- [10] A. K. Geim, *Nobel Lecture: Random walk to graphene*, Rev. Mod. Phys, **83**, 851 (2011).
- [11] T. Heinzel *Mesoscopic Electronics in Solid State Nanostructures*, Wiley, Weinheim (2007).
- [12] P. Hohenberg, W. Kohn, *Inhomogenous electron gas*, Phys. Rev. **136**, B864 (1964).
- [13] M. I. Katsnelson, K. S. Novoselov, A. K. Geim, *Chiral tunnelling and the Klein paradox in graphene*, Nature Physics **2**, 620 - 625 (2006).
- [14] W. Kohn, L. J. Sham, *Self-consistent equations including exchange and correlation effects*, Phys. Rev. **140**, A1133 (1965).
- [15] K. Lier and R. R. Gerhardts, *Self-consistent calculations of edge channels in laterally confined two-dimensional electron systems*, Phys. Rev. **B 50**, 7757 (1994).
- [16] P. Marconcini, M. Macucci, *The $k \cdot p$ method and its application to graphene, carbon nanotubes and graphene nanoribbons: the Dirac equation*, La Rivista del Nuovo Cimento **45** (8-9), 489-584 (2011)

- [17] R. M. Martin, *Electronic Structure*, Cambridge University Press, Cambridge, (2004).
- [18] E. McCann, M. Koshino, *The electronic properties of bilayer graphene*, Rep. Prog. Phys. **76** 056503 (2013).
- [19] E. Merzbacher, *Quantum Mechanics*, Wiley, (1998).
- [20] K. S. Novoselov, V. I. Fal'ko, L. Colombo, P. R. Gellert, M. G. Schwab, K. Kim, *A roadmap for graphene*, Nature **490**, 192 (2012).
- [21] K. S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, A. A. Firsov, *Electric Field Effect in Atomically Thin Carbon Films*, Science **306**, 666 (2004).
- [22] K. S. Novoselov, *Nobel Lecture: Materials in the Flatland*, Rev. Mod. Phys, 83, 837 (2011).
- [23] K. S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, A. A. Firsov, *Electric Field Effect in Atomically Thin Carbon Films*, Science **306**, 666 (2004).
- [24] J. H. Oh, R. R. Gerhardtts, *Self-consistent Thomas-Fermi calculation of potential and current distributions in a two-dimensional Hall bar geometry*, Phys. Rev. **B 56**, 13519 (1997).
- [25] A. I. Rahachou, I. V. Zozoulenko, *Light propagation in finite and infinite photonic crystals: The recursive Green's function technique* Phys. Rev **B 72**, 155117 (2005).
- [26] A.V. Rozhkov, G. Giavaras, Y. P. Bliokh, V. Freilikher, F. Nori, *Electronic properties of mesoscopic graphene structures: Charge confinement and control of spin and charge transport*, Physics Reports, **503**, 77-114 (2011).
- [27] A. A. Shylau, J. W. Klos, I. V. Zozoulenko, *Capacitance of graphene nanoribbons*, Phys. Rev. **B 80**, 205402 (2009).
- [28] H. Xu, T. Heinzl, and I. V. Zozoulenko, *Edge disorder and localization regimes in bilayer graphene nanoribbons*, Phys. Rev. **B 80**, 045308 (2009).
- [29] H. Xu, T. Heinzl, M. Evaldsson, and I. V. Zozoulenko, *Magnetic barriers in graphene nanoribbons: Theoretical study of transport properties*, Phys. Rev. **B 77**, 245401 (2008).

Papers

The articles associated with this thesis have been removed for copyright reasons. For more details about these see:

[http://urn.kb.se/resolve? urn:nbn:se:liu:diva-136093](http://urn.kb.se/resolve?urn:nbn:se:liu:diva-136093)