

École polytechnique de Louvain

Electron optics in graphene

Authors : **Quentin Chardon**, **Raphaël Vereecken**

Supervisor : **Benoit Hackens**

Readers : **Jean-Christophe Charlier**, **VINCENT Bayot**

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Abstract

Since the discovery of the Quantum Hall effect in 1980, electronic interferometry took a significant leap forward thanks to localized edge states topologically protected and demonstrating mesoscopic coherence length. More recently the synthesis of graphene and the development of van der Waals heterostructures have been crucial to overstep drawbacks of semiconductor heterojunctions and taking advantage of graphene properties.

This work is at the crossroads of these major discoveries or breakthroughs. It focuses on different ways to generate electronic interferences in Quantum Hall regime of graphene by the mean of a scanning gate microscope (SGM) to locally modify the electronic bands. This thesis is split in three axis to tackle the subject. In first instance, simulations with Kwant to explore the coupling between edge states and an external potential while observing different patterns of interference with different designs of graphene Hall bar. Thereafter, the fabrication in laboratory of the graphene heterostructure from scratch. Finally, an analysis of experiment data to compare simulations to real world conditions.

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List of Symbols

Abbreviations

2DEG	Two-Dimensional Electron Gas
AFM	Atomic Force Microscopy
Al	Aluminum
As	Arsenic
BN	Boron Nitride
CCD	Charge Coupled Device
CVD	Chemical Vapor Deposition
DFT	Density Functional Theory
EBPVD	Electron Beam Physical Vapor Deposition
ES	Edge State
FF	Filling Factor
FP	Fabry-Pérot
Ga	Gallium
In	Indium
LL	Landau Level
MIBK	Methyl Isobutyl Ketone
MZI	Mach-Zehnder Interferometer
O ₂	Dioxygen
PDMS	Polydimethyl Siloxane
PPC	Polypropylene Carbonate
QHE	Quantum Hall Effect
QHI	Quantum Hall Island
QPC	Quantum Point Contact
RTA	Rapid Thermal Annealing
SGM	Scanning Gate Microscope
Si	Silicon
SiC	Silicon Carbide
SiO ₂	Silicon Oxide
vdW	van der Waals

Physical quantities

$\hbar$	Reduced Plank constant
λ	Wavelength
ρ_{xy}	Hall resistivity
ω_c	Cyclotron frequency
τ	Time between two collisions
$\hat{\Pi}$	Kinetic momentum operator
ξ	Valley pseudospin
σ	Pauli matrices
ν	Filling factor
σ	Conductivity
a_G	graphene lattice parameter
$\hat{\mathbf{A}}$	Magnetic vector potential
$\hat{a}$ and $\hat{a}^\dagger$	Ladder operators
B_{field}	Magnetic field
E	Electric field
e	Electrical charge
$\mathcal{H}$	Hamiltonian
$\mathcal{H}_D^\xi$	Hamiltonian for Dirac fermions
$\mathcal{H}^{eff}$	Effective hamiltonian
I_x	Current along x-axis
J_x	Current density along x-axis
l_0	Magnetic length
m^*	Effective mass
n	Landau level index
n_B	Magnetic flux density
n_e	Electronic density
$\hat{\mathbf{p}}$	Canonical momentum operator
R_{xx}	Longitudinal resistance
R_{xy}	Hall resistance
r_n	'Classical radius' of edge channel
s	Scalling parameter
t	Hopping parameter
V_{eff}	Effective potential
v_F	Fermi velocity
v_x	Drift velocity

Chapter 1

Introduction

It is fair to say that interferometry has always passionated physicists and led to reconsider physics that scientists knew at their time. The most striking example is probably Young's double-slit experiment that highlighted the wave behavior of light [1]. Nowadays, interferometry techniques are used in virtually every scientific field from quantum mechanics to astronomy. It is a powerful tool of experiment allowing to measure data or to verify physical models.

Another important breakthrough was in 1928 when the Davisson–Germer experiment demonstrated the wave-like character of electrons [2]. From this observation, surface determination techniques such as low-energy electron diffraction [3] have been developed or more recently, the craze about quantum computing with quantum operations on electronic wave function [4].

It can be interesting to implement directly the interferometer in mesoscopic materials rather than in free space. In this case, the interfering electrons are the free electrons of the material. This kind of setups can help to explore properties of the material itself or to create for instance Cooper pair box for charge quantum bits [5]. However, for the experiment to make sense, the electrons (or holes) need to follow well-defined paths and the experimenters need to have control on the trajectories followed by the charge carriers. This is the reason why quantum Hall regime is particularly attractive in electronic interferometers.

The quantum Hall effect (QHE) has been discovered in 1980 by the German physicist Klaus von Klitzing [6]. It occurs in 2D electronic systems at low temperatures and strong perpendicular magnetic fields. Since its discovery, it has raised particular interest in many studies, mainly because of the quantification and localization of electronic channels. Those so-called edge states can be manipulated by varying the electrostatic landscape and their coherence length are of the order of more than 10 micrometers [7]. Therefore, efforts have been multiplied since to design and implement interferometers such as Mach-Zehnder or Fabry-Pérot using the charge carriers of the edge states.

At first, these interferometers were implemented from 2D electron gas made from semiconductors generally based on GaAs. Part of these studies have refocused their interest on graphene when it has been first produced in 2004 [8]. Indeed, this new 2D material demonstrating impressive electrical, mechanical and optical properties is now commonly used for electronic interferometry.

In this context, the purpose of the thesis is to explore different geometries and setups to highlight different interference patterns in the quantum Hall regime of graphene. Analyzing at a local scale the working principle of electron interferometry with a scanning gate microscope (SGM) is also a burning issue. To this end, this work is divided in the following chapters:

- A **State of the art** where theoretical information are given about graphene and heterostructures in general, mathematical and phenomenological description of the quantum Hall effect and setup details for electronic interferometers.
- **Simulations** of different designs of graphene Hall bars to retrieve Aharonov-Bohm resistance oscillations in the quantum Hall regime with various sets of parameters.
- The **Fabrication process** of the heterostructure from graphene exfoliation to the completion of the device.
- Experimental data analysis in **InGaAs/InAlAs electronic interferometer** to compare with the simulations.

Chapter 2

State of the art

This chapter is written to give the reader a comprehensive view of the building blocks at stake in the devices built and simulated.

The following sections are divided in three main axis that aim to answer these questions:

- What are the basic materials used and what are their properties ?
- How charge carriers are spatially localized and how they are flowing in these materials under a particular quantum regime ?
- How to build an electronic interferometer where the charge carriers interfere with themselves in the material ?

This begins by introducing the concept of van der Waals heterostructure. Then, the materials that assembled in the heterostructure are detailed. Especially graphene as it is the conductor material where the electronic interferometry takes part.

Afterwards, the quantum Hall effect is explained and mathematically described. Also, Aharonov-Bohm effect arising from the quantum Hall regime is detailed. Finally, optical and electronic interferometers are introduced as well as a review of a recent paper on Fabry-Pérot interferometer in graphene.

A supplementary section on InGaAs/InAlAs semiconductor heterostructure as experimental data from the same regime will be discussed.

2.1 Van der Waals heterostructure

2.1.1 General description

In recent years, extensive researches on graphene and other 2D atomic crystals have been done. It lead to a better understanding and discovery of new properties in the field of material sciences. In parallel with the studies on 2D materials, another field has emerged in the past 10 years or so: materials by design [9]. The idea is to combine different materials with different properties in order to build a "super" functional material. However, this is no easy task. At this time, there is no global solution to mix and match any crystals.

The actual best methods that had proven their effectiveness are van der Waals stacking, physical

epitaxy and chemical vapor deposition. The first technique will be developed in this section.

A van der Waals (vdW) heterostructure can be defined as multiple atomic or molecular planes stacked layer by layer in a precisely chosen sequence like shown on Figure 2.1. It's called van der Waals heterostructure because of the weak distance-dependent force bounding atoms and molecules. Without entering the quantum physics, it corresponds to the electrostatic interaction between induced and/or permanent electrical dipoles. Increasing the distance of the interaction makes the intensity of the force vanish quickly. Indeed, the force is inversely proportional to the distance d . Strong covalent bonds provides in-plane stability of 2D crystals whereas relatively weak vdW-like forces are sufficient to keep the stack together.

The big asset that differentiate vdW heterostructure with classical semiconductor heterojunctions is that there are no constraints of lattice matching between layers or other material incompatibilities [10].

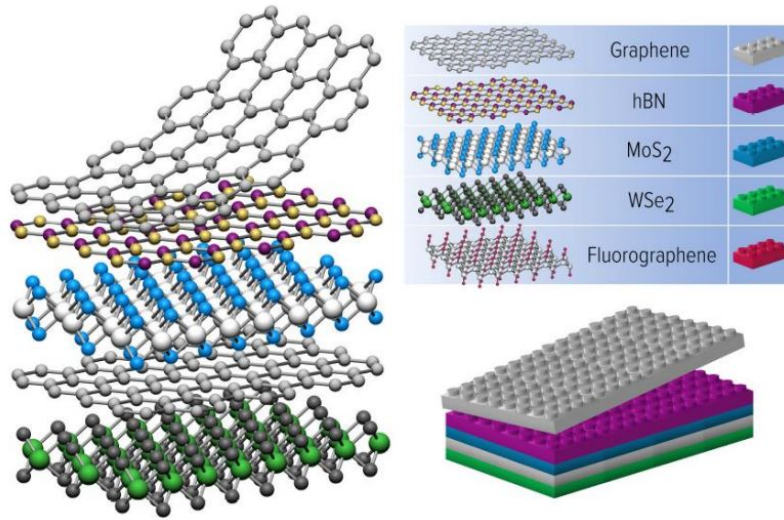


Figure 2.1: Example of van der Waals heterostructure with two layers of graphene, one of hBN, one of MoS₂ and one of WSe₂. A simple approach to understand vdW heterostructure is to represent every 2D crystal as a building Lego block that can stack above each other. [11]

In the context of this work, the vdW stacking is the key to protect the basic block of this study: graphene.

2.1.2 Graphene

Crystal structure

The Figure 2.2 a) represents a view of the graphene lattice. It consists of a two dimensional honeycomb lattice composed of carbon atoms. Since it is not possible to represent a honeycomb structure with one Bravais lattice, two lattices are needed. The first one is represented by black dots and the second one by white dots. Graphene is a single layer of graphite and the distance between two nearest neighbor carbon atoms (between a black dot carbon and a white dot carbon in Figure 2.2 a)) is $D = 1.42 \text{ \AA}$. The primitive unit cell has basis vectors: $\vec{a}_1 = \frac{D}{2}(3, \sqrt{3})$ and $\vec{a}_2 = \frac{D}{2}(3, -\sqrt{3})$. In that case, one can obtain the lattice parameter $a_G = 2.46 \text{ \AA}$.

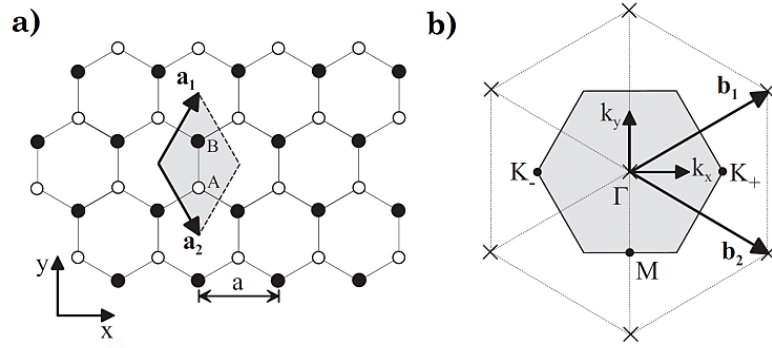


Figure 2.2: a) A 2-dimensional crystal structure for graphene with $\vec{a}_1$ and $\vec{a}_2$ basis vectors for the primitive unit cell, a the lattice parameter and A, B carbon atoms. The lattice is divided in two sub-lattices (white atoms and black atoms). The grey area represents the unit cell. b) The reciprocal lattice of graphene with $\vec{b}_1$ and $\vec{b}_2$ basis vectors. The grey area represents the first Brillouin zone [12].

On Figure 2.2 b), the first Brillouin zone is highlighted in grey. It has three high symmetrical points Γ , M and K.

Orbital structure

The representation of orbitals is shown on Figure 2.3. Carbons are linked to 3 nearest neighbors and hence present sp^2 hybridized orbitals, depicted in blue. There is still one electron per atom that is oriented perpendicularly to the plane in the p_z orbital, depicted in light pink. Thanks to that configuration, a two-dimensional electron gas (2DEG) is created.

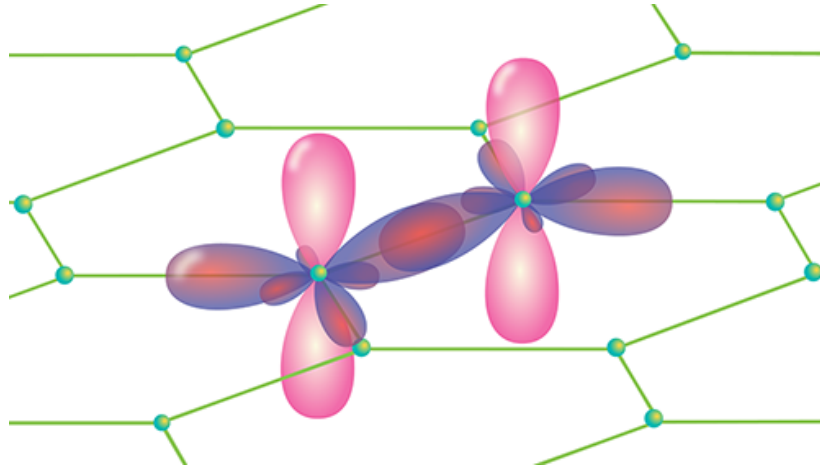


Figure 2.3: Representation of graphene orbitals. In light pink it is the $2p_z$ and in blue sp^2 hybridized orbitals. The carbon atoms are represented in green [13].

Band structure

The band structure is represented on Figure 2.4. One can observe that the conduction and valence bands intercept each other at K points. More precisely, on K_- and K_+ thereby forming Dirac cones. Graphene is categorized as a zero band gap semiconductor. An interesting thing to notice is on the

Figure 2.4 b) which focuses on the interception of the two energy bands. One can remark that the dispersion of energy is linear as shown in the Equation 2.2. It means that free charge carriers are associated to massless particles. In the vicinity of the Dirac cone, electrons and holes in graphene are no more described by the Schrödinger equation but by the Dirac equation which takes account of relativist theory.

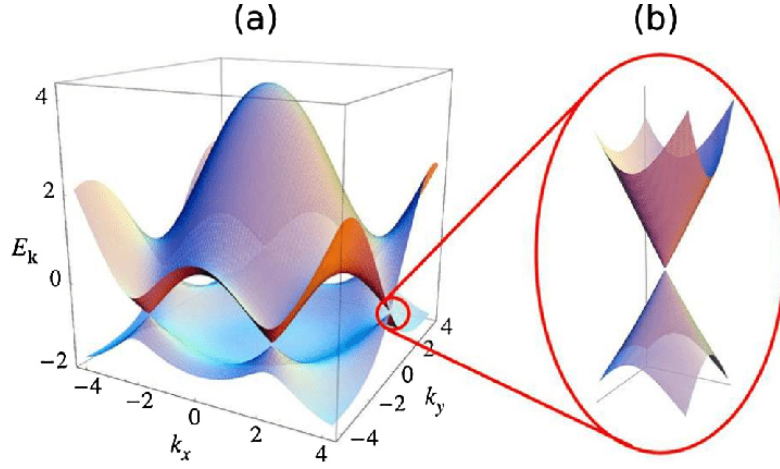


Figure 2.4: a) Band structure of graphene showing Dirac point between π and π^* bands at K points. b) Zoom on bands contact to show the Dirac cone. [14]

Mathematically, it is possible to compute energy bands represented here above. It is done by using tight binding models, detailed in section 3.1. Thereby, the energy can be expressed with the following equation:

$$E_{\pm}(\mathbf{k}) = \pm t \sqrt{1 + 4 \cos^2(\sqrt{3}k_x a) + 4 \cos\left(\frac{\sqrt{3}}{2}k_x a\right) \cos\left(\frac{3}{2}k_y a\right)} \quad (2.1)$$

with t the hopping parameter. The expression 2.1 can be developed in Taylor series near the points $\mathbf{k} = K_+ + \delta\mathbf{k}$ and $\mathbf{k} = K_- + \delta\mathbf{k}$ that corresponds to the confluence of the conduction and valence bands. Due to the additional degree of freedom concerning K points (K_+ and K_-), one can introduce the concept of valley which behaves like pseudo-spin ξ . Finally, one may obtain the following equation:

$$E_{\pm}(\mathbf{k}) \approx \pm \hbar v_F |\mathbf{k}| \quad (2.2)$$

with $v_F = \frac{3ta}{2\hbar}$ the electronic group velocity which is expected to be around 10^6 m/s in graphene. [15]

There are other remarkable consequences of the linear dispersion in graphene:

- The first one is the density of state (DOS) function according to the energy. On Figure 2.5, one can notice that it is linear between $-\frac{t}{2}$ and $\frac{t}{2}$ corresponding to the energy limits such that the linear dispersion of energy is valid.
- Another consequence is the tunability of the charge carriers. Indeed, Figure 2.6 shows the evolution of resistivity when a gate voltage V_g is applied. The current of charge carriers can be changed instantly because of the zero band gap between valence and conduction bands. When increasing V_g , the Fermi energy increases and passes from the valence to the conduction bands. Thereby, it is possible to switch from electron to holes current continuously.

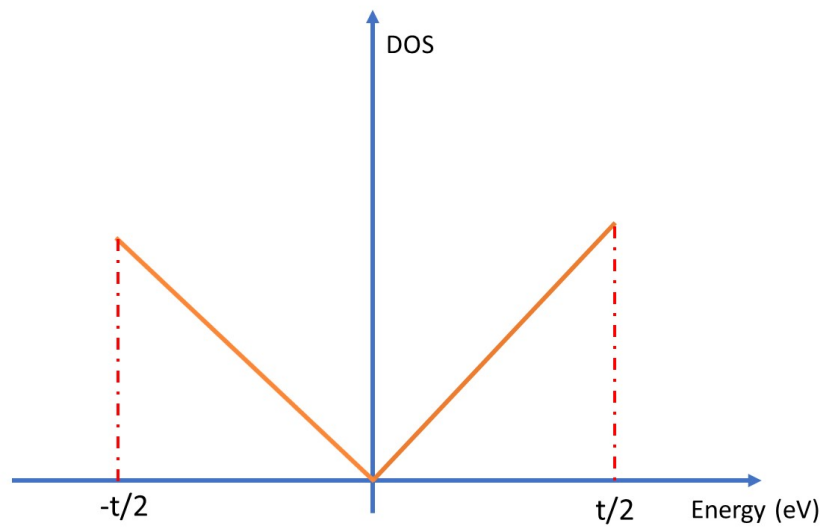


Figure 2.5: Linear density of state for graphene between $-t/2$ and $t/2$ which corresponds to the linear regime of graphene.

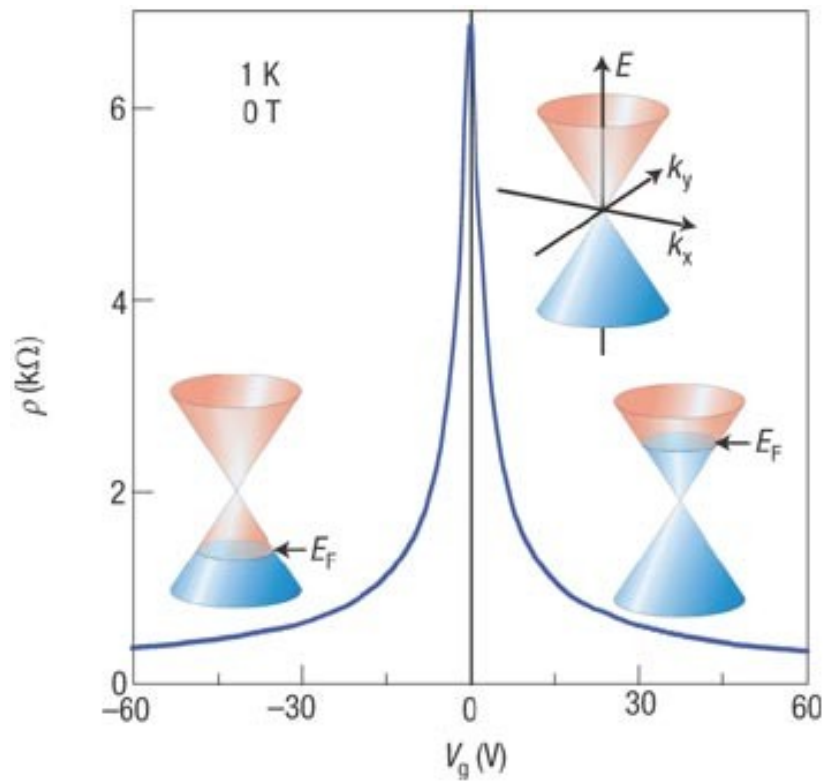


Figure 2.6: Resistivity as a function of V_g . By increasing V_g , the Fermi energy is increasing too, allowing to switch from electron to holes currents continuously [16].

Other properties

Graphene has a lot of other astonishing properties like mechanical properties or optical properties [17]. Here is a non-exhaustive list of some examples:

- Thermal conductivity between 3000 to 5000 W/mK.
- Toughest 2D materials in term of tensile strength. About 1 Tpa.
- Light material, about 0.77 milligrams per square meter.
- Very stretchable, around 20 % of its initial size.
- Can be used to make solar cells because it absorbs 2.3 % of white light.

2.1.3 Hexagonal boron nitride

Boron nitride (BN) is a material that can be found in various crystalline forms. Hexagonal boron nitride (hBN) is the most stable one and the most beneficial in the frame of this work. Indeed, it exhibits a similar structure as graphene. Besides being hexagonal, hBN is also a honeycomb lattice. The in-plane bonds between boron and nitrogen are covalent whereas the layers are maintained together by weak vdW forces. Its structure is represented on Figure 2.7

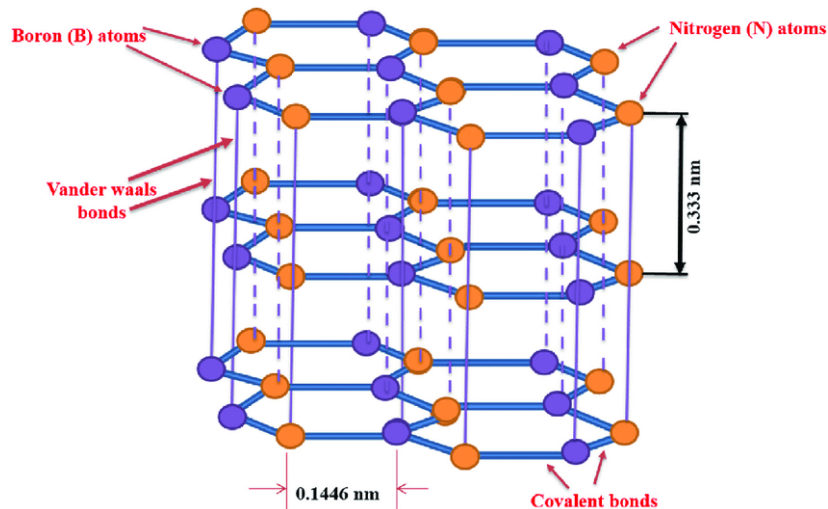


Figure 2.7: 3D view of hBN crystal structure. Orange dots are nitrogen atoms and purple ones are boron atoms connected together via covalent bonds [18].

Moreover, there is only a lattice mismatch of 1.8% between lattice constant of graphene a_G and lattice parameter of hBN a_{hBN} [19]. Concerning its surface, it is ultra-flat and free of dangling bonds. Therefore, it is the perfect candidate to encapsulate graphene with. The benefit of this stacking is to protect graphene from outside dust/stimuli and to isolate it electrically. Indeed, hBN in its electronic structure is a wide band gap insulator with a band gap equal to 5.2 eV.

2.2 Quantum Hall Effect

2.2.1 Hall effect

The Hall effect has been brought to light in 1879 by E. H. Hall where he measured the apparition of a potential proportional and perpendicular to the current and to the magnetic field in a material.

In a conductor, the current along the x-axis I_x is given by:

$$I_x = J_x w t = n q v_x w t \quad (2.3)$$

where J_x is the current density along the x-axis, n the charge carrier number density, v_x the drift velocity of these carriers, w and t respectively the width and thickness forming the area intercepted by I_x .

By applying the Lorentz force in the steady state ($\mathbf{F} = \mathbf{0}$), the direction of the resulting electric field is found:

$$\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}) = \mathbf{0} \quad (2.4)$$

$$\Leftrightarrow \begin{pmatrix} 0 \\ E \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ -v \cdot B \\ 0 \end{pmatrix} \quad (2.5)$$

The electric field is actually transverse to the carrier current and the magnetic field. Figure 2.8 represents a classic Hall bar experiment where the voltage difference is applied along the x-axis and the magnetic field is along the z-axis. In particular, interesting parameters to compute are the Hall

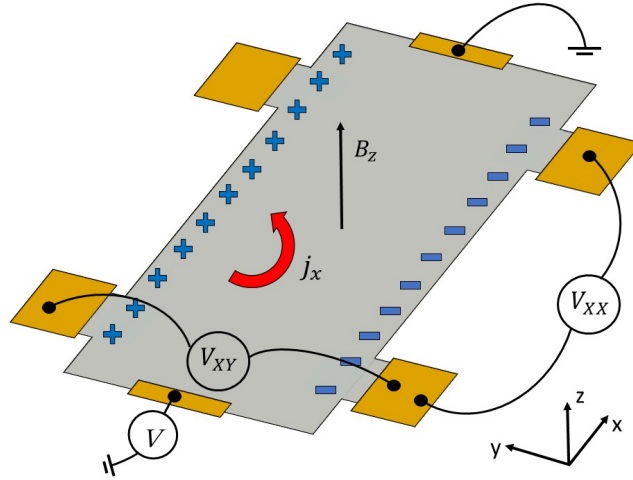


Figure 2.8: Typical six-terminal Hall bar is used in experiments. The voltage drop is applied on the x-axis with the magnetic field along the z-axis. The blue symbols represent the accumulation of charges inducing the electric field along the y-axis.

resistivity (or transverse resistivity) ρ_{xy} [20] :

$$\rho_{xy} \equiv \frac{E_y}{j_x} = \frac{B_z}{en_e} \quad (2.6)$$

and the longitudinal resistivity ρ_{xx} :

$$\rho_{xx} \equiv \frac{E_x}{j_x} = \frac{m}{ne^2\tau} \quad (2.7)$$

which leads to the conclusion that only the Hall resistivity is proportional to the magnetic field magnitude.

2.2.2 General description on QHE

The quantum Hall effect (QHE) occurs in 2D electronic systems at generally lower temperatures and stronger magnetic fields ($\omega_c \tau \gg 1$, with ω_c the cyclotron frequency and τ the time between two collisions) than classical Hall effect. Since the discovery, it has been extensively studied. One reason for this enthusiasm is the scalability of this phenomenon. Indeed, QHE is one of the few quantum mechanical effect which is measurable at a macroscopic level [21]. Another key feature of the QHE is the exact quantization of the transverse Hall resistance R_{xy} in units of e^2/h . This resistance demonstrates predictable clean plateaus which are immune, up to certain level, to disorder in the system. These quantized R_{xy} are matching with zero longitudinal resistance R_{xx} [22]. This is a major difference with the classical Hall effect.

2.2.3 Non-relativistic Landau levels

This section is inspired by [21]:

When a strong magnetic field is applied to a 2D electron gas, their energy quantized. The development of this section is based on the Drude model [23]. This model considers a free electron gas; the influence of the nuclei potentials is then neglected. The magnetic field B_z is oriented along the z -axis. The movement of electrons is only considered along the coordinates x and y , perpendicular to the magnetic field because the magnetic field has no effect in the z -axis movement of charge carriers in a narrow semiconductor quantum well.

The Hamiltonian of a free electron is given by $\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m}$. When the magnetic field is applied to the system, the Peierls substitution is used [24] [25] to replace canonical momentum $\hat{\mathbf{p}}$ by the gauge-invariant kinetic momentum $\hat{\Pi}$:

$$\hat{\mathbf{p}} \longrightarrow \hat{\Pi} = \hat{\mathbf{p}} + e\hat{\mathbf{A}}(\mathbf{r}) \quad (2.8)$$

where $\hat{\mathbf{A}}$ is the magnetic vector potential. The Hamiltonian of an electron in a magnetic field then becomes:

$$\mathcal{H} = \frac{\hat{\Pi}^2}{2m} = \frac{1}{2m}(\hat{\mathbf{p}} + e\hat{\mathbf{A}}(\mathbf{r}))^2 \quad (2.9)$$

The Hamiltonian can be rewritten considering only the x and y components of displacement as discussed above:

$$\mathcal{H} = \frac{(\hat{\Pi}_x + \hat{\Pi}_y)}{2m} \quad (2.10)$$

With no magnetic field, the momentum operators $\hat{p}_x$, $\hat{p}_y$ and $\hat{p}_z$ commute with each other as for instance : $[\hat{p}_x, \hat{p}_y] = 0$. It is not true anymore with $B \neq 0$, the commutation relation between Π_x and Π_y is given by:

$$[\hat{\Pi}_x, \hat{\Pi}_y] = -ie\hbar \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) = ie\hbar B_z \quad (2.11)$$

One can introduce the ladder operators, $\hat{a}$ and $\hat{a}^\dagger$ [25]:

$$\hat{a} = \frac{l_0}{\sqrt{2\hbar}}(\hat{\Pi}_x - i\hat{\Pi}_y), \quad \hat{a}^\dagger = \frac{l_0}{\sqrt{2\hbar}}(\hat{\Pi}_x + i\hat{\Pi}_y) \quad (2.12)$$

where

$$l_0 \equiv \sqrt{\frac{\hbar}{eB_z}} \quad (2.13)$$

is the magnetic length. Concerning a and $a^\dagger$, they represent a complex gauge-invariant momentum and are helpful to extract energy eigenvalues. They are normalized for the commutation relation to be:

$$[\hat{a}, \hat{a}^\dagger] = 1 \quad (2.14)$$

It is convenient to flip the Equations [2.12](#):

$$\hat{\Pi}_x = \frac{\hbar}{\sqrt{2}l_0}(\hat{a}^\dagger + \hat{a}), \quad \hat{\Pi}_y = -i\frac{\hbar}{\sqrt{2}l_0}(\hat{a}^\dagger - \hat{a}) \quad (2.15)$$

These expressions of gauge-invariant kinetic momentum can be substitute in Hamiltonian Equation [2.10](#):

$$\mathcal{H} = \frac{\hbar^2}{4ml_0^2} \left(2(a^\dagger a + a a^\dagger) \right) \quad (2.16)$$

$$= \frac{\hbar^2}{4ml_0^2} \left(4a^\dagger a + 2[a, a^\dagger] \right) \quad (2.17)$$

with $a^\dagger a = n$ the number operator and $[a, a^\dagger] = 1$. Finally, the eigenvalues of the Hamiltonian are:

$$E_n = \frac{\hbar^2}{ml_0^2} \left(n + \frac{1}{2} \right) \quad \text{with } n \in [0, 1, 2, \dots] \quad (2.18)$$

These quantized energies are called the Landau levels (LL). The energy difference between two levels is proportional to the magnetic field magnitude B as $l_0^2 \propto 1/B$. The Figure [2.9](#) a) represents the LLs as a function of B .

2.2.4 Relativistic Landau levels

The main focus on this work is based on graphene. As it is stated in section [2.1.2](#), charge carriers near the Fermi level are modeled as Dirac fermions.

Let's start by reconsidering the new Hamiltonian for Dirac fermions without magnetic field first [\[26\]](#):

$$\mathcal{H}_D^\xi = \xi v_F \boldsymbol{\sigma} \cdot \hat{\mathbf{p}} \quad (2.19)$$

with $\xi = \pm 1$ the valley pseudospin due to the two fold valley symmetry of the K and K' points [\[26\]](#) and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ the Pauli matrices that are given by:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (2.20)$$

Including the effect of the magnetic field, the Peierls substitution of Equation [2.8](#) is required and the Dirac Hamiltonian becomes:

$$\mathcal{H}_D^\xi = \xi v_F \begin{pmatrix} 0 & \hat{\Pi}_x - i\hat{\Pi}_y \\ \hat{\Pi}_x + i\hat{\Pi}_y & 0 \end{pmatrix} \quad (2.21)$$

The kinetic momentum $\hat{\Pi}$ are written in terms of the ladder operators:

$$\mathcal{H}_D^\xi = \xi \sqrt{2} \frac{\hbar v_F}{l_0} \begin{pmatrix} 0 & \hat{a} \\ \hat{a}^\dagger & 0 \end{pmatrix} \quad (2.22)$$

There are two components for the eigenvector ψ_n of $\mathcal{H}_D^\xi$ because of the two sublattices A and B :

$$\psi_n = \begin{pmatrix} \phi_n^A \\ \phi_n^B \end{pmatrix} \quad (2.23)$$

One need to solve the eigenvalues E_n of the system:

$$\frac{\sqrt{2}\hbar v_F}{l_0} \cdot \begin{pmatrix} \hat{a}\phi_n^B \\ \hat{a}^\dagger\phi_n^A \end{pmatrix} = E_n \begin{pmatrix} \phi_n^A \\ \phi_n^B \end{pmatrix} \quad (2.24)$$

By substitution, the relation for sublattice B is given by:

$$\hat{a}^\dagger \hat{a} \phi_n^B = \frac{1}{2} \left(\frac{E_n l_0}{\hbar v_F} \right)^2 \phi_n^B \quad (2.25)$$

where $\hat{a}^\dagger \hat{a}$ is the occupation number operator $\hat{n}$. Isolating E_n gives:

$$E_n = \pm \frac{\sqrt{2n} v_F \hbar}{l_0} \quad (2.26)$$

It is convenient to rewrite this expression with l_0 developed (Equation 2.13):

$$E_n = \pm v_F \sqrt{2\hbar e} \sqrt{nB_z} \quad \text{with } n \in [0, 1, 2, \dots] \quad (2.27)$$

In comparison with non-relativistic Equation 2.18 where $E_n \propto nB$, the relativist case is $E_n \propto \sqrt{nB}$. Besides positive E_n values associated to electron conduction (blue curves in Figure 2.9 b)), there are symmetrically negative E_n values associated with hole conduction (red curves in Figure 2.9 b)). The zero energy LL ($n = 0$) is shared by both electrons and holes.

2.2.5 Edge states (ESs)

This section is inspired by [4]:

In solid-state physics, the relative position of the Fermi level with the electronic bands determines if there is electronic conduction or not. Indeed, the Fermi level is the highest energy level occupied by electrons at 0 K. To have a current flowing in the material, the Fermi level has to lay inside an electronic band: it is called a partially occupied band.

If a material demonstrates no disorder or any external local perturbation, the LL (Equation 2.27) are flat in the central area. To conduct current, a LL has to be perfectly align with the Fermi level. Otherwise, when the Fermi energy lays in the energy gap between two LLs, the material behaves like an electric insulator. It is indeed a fragile tuning which is not suitable for precise electron transmission along a defined path. Fortunately, current can propagate in the edges of the material thanks to the confining potential. As a matter of fact, this confining potential is behaving like an energetic barrier due to ending of the lattice on the edges. It bends the LLs upward and allows intersections with

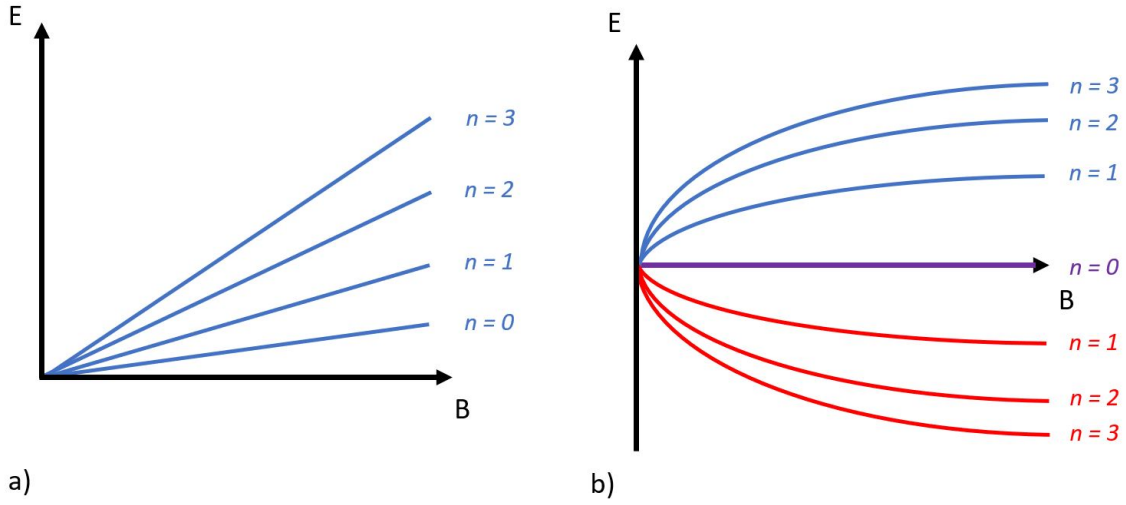


Figure 2.9: Evolution of LLs as a function of B . (a) Relativistic case. The energetic spacing between LLs is proportional to B . (b) Non-relativistic case. The energetic spacing between LLs is proportional to $\sqrt{B}$.

the Fermi energy (Figure 2.10). These intersections create and position what is called edge channels. The width of these channels corresponds to the spatial extent of the wave function associated to the LLs and it is of the order of l_0 introduced in Equation 2.13:

$$r_n = l_0 \sqrt{2n+1} \quad (2.28)$$

where r_n is the 'classical radius' of the channel. It is worth noting that the higher LL index n , the larger the channel is.

Concerning the confinement potential V_{ext} , two separate cases have to be distinguished [27]:

- If V_{ext} varies slowly in comparison with l_0 : it corresponds to a smooth external potential at the edges. The energy levels simply follow V_{ext} at the edge. For instance, this model is used in 2DEG of GaAs heterostructures.
- If V_{ext} varies quickly in comparison l_0 : it corresponds to an abrupt external potential at the edges. The energy profile is exactly the same for all levels and the LL start to increase at a distance depending on n , of the order of $\sqrt{2n+1}l_0$ from the boundary. For instance, this model is used in graphene ribbons because of the sharp boundaries of graphene. This is the model studied in the following developments.

The filling factor (FF), ν , is introduced here. It is a parameter that will be necessary for the following sections. It corresponds to the ratio between the electronic density n_e and the flux density n_B :

$$\nu = \frac{n_e}{n_B} = \frac{\hbar n_e}{eB} \quad (2.29)$$

Expressing it otherwise, it is the number of completely filled LLs below the Fermi level. There are many ways to vary ν in the material: varying B , locally gate a region of choice with a local potential or applying a back-gate voltage.

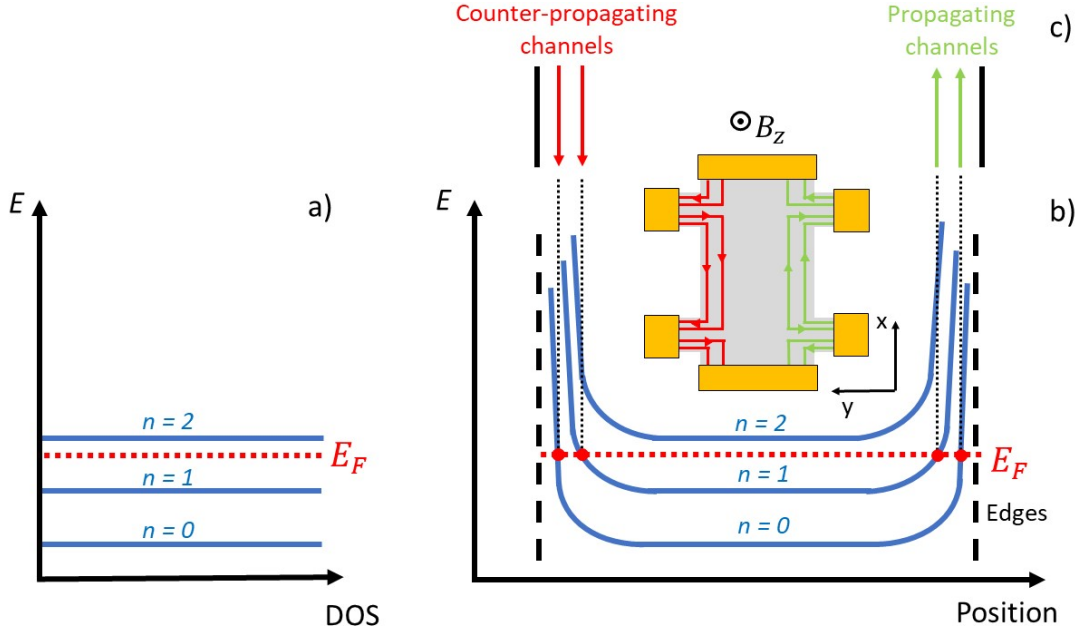


Figure 2.10: (a) Schematic representation of the three first LLs with the Fermi energy laying between $n = 1$ and $n = 2$. These LLs are spaced by energy gap of $\hbar\omega_c$. (b) LLs bent by the confinement potential which induce intersections with the Fermi level on the edges. (c) Each intersection lead to the apparition of a new conduction edge channel. The green channels are the propagating ones while the red channels on the other side are counter-propagating the current. However, the bulk remains an insulator.

It is important to pay attention if the material has been prepared properly or not (i.e. in classic semiconductors, dopants trapped in the material and located close to the two-dimensional gas). In the second case, a disorder potential appears on the material representing these "defects". According to these variations of potential, the Fermi level can be intersected locally where it didn't with no disorder. LLs are indeed broadened in this case (see Figure 2.11).

The disorder on the ESs can also contribute to undesirable effects. Depending on the magnitude of the magnetic field and the degree of disorder, electrons in channels could interact with each other. They could also be redirected in the bulk and therefore undergo scattering. The interesting properties of the ESs would be lost.

The following inspection of the ESs is made on a 2DEG non-relativistic.

To derive mathematically the concept of ESs, let's confine the 2DEG in an external potential $V_{ext}(x)$. This potential is only function of the x coordinate with a vector potential $\mathbf{A}$ chosen as $\mathbf{A} = (0, Bx, 0)$ [4].

The new Hamiltonian is given by adding to the previous one the $V_{ext}(x)$ term:

$$\mathcal{H} = \frac{\hat{H}^2}{2m^*} = \frac{1}{2m^*}(\hat{\mathbf{p}} + e\hat{\mathbf{A}}(\mathbf{r}))^2 + V_{ext}(x) \quad (2.30)$$

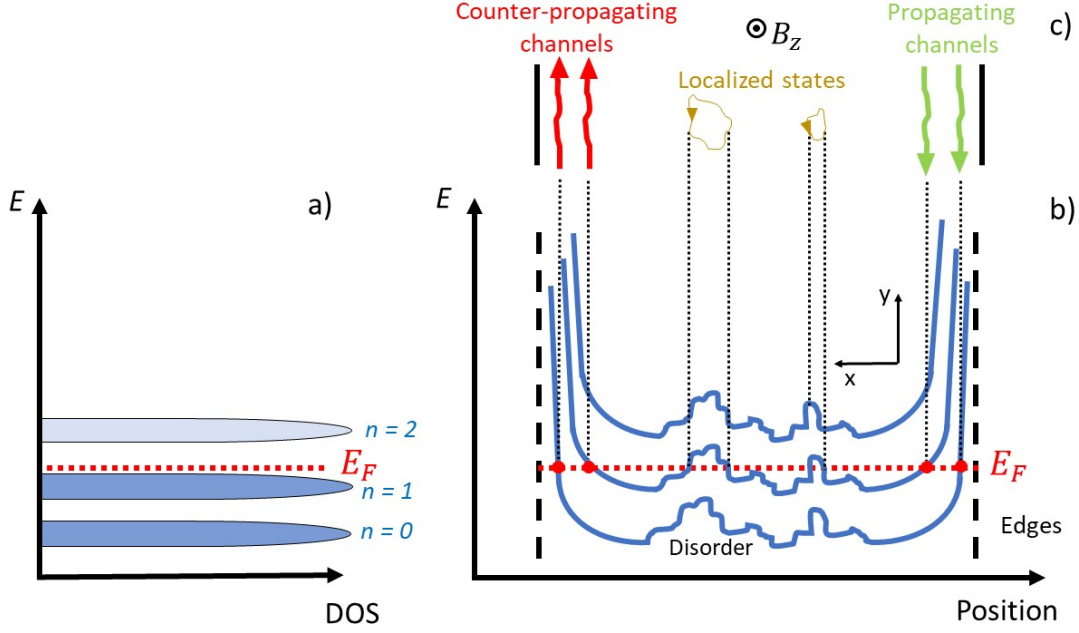


Figure 2.11: (a) The Landau levels are broadened under the effect of the disorder potential. (b) and (c) The local effect of the disorder implies loop of current that does not conduct charge carriers along the material.

The impulsion operator is rewrite with its definition : $\hat{\mathbf{p}} = -i\hbar\nabla$ and likewise for the vector potential:

$$\mathcal{H} = \frac{1}{2m^*} \left(-\hbar^2 \frac{\partial^2}{\partial x^2} + \left(-\hbar^2 \frac{\partial^2}{\partial y^2} - 2i\hbar e B x \frac{\partial}{\partial y} \right) + e^2 B^2 x^2 \right) + V_{ext}(x) \quad (2.31)$$

Quantum mechanics tells us that the impulsion operator in a direction (i.e. y for instance) commute with the Hamiltonian: $[\hat{P}_y, \hat{H}] = 0$. The corresponding eigenvalues with wave vector k and Landau level index n is:

$$\Psi_{n,k}(x, y) = \varphi_n(x, k) e^{iky} \quad (2.32)$$

It's composed of a plane wave part e^{iky} which is in free motion along y -axis and a transverse part $\varphi_n(x, k)$ along the x -axis. The latter is called ES and it's in fact the eigenfunction of $\mathcal{H}$ taken for the x -axis (Figure 2.12 b) for the representation of the ESs along the x -axis). This Hamiltonian is called $\mathcal{H}^{eff}$ and is given by:

$$\mathcal{H}^{eff}(k) = \frac{-\hbar^2}{2m^*} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m^* \omega_c^2 \left(x + \frac{\hbar}{eB} k \right)^2 + V_{ext}(x) \quad (2.33)$$

where $\omega_c = eB/m^*$ is the cyclotron frequency. One can rewrite the last two terms representing the parabolic contribution and the well-shaped potential V_{ext} as V_{eff} :

$$V_{eff}(x) = \frac{1}{2} m^* \omega_c^2 (x - x_0)^2 + V_{ext}(x) \quad (2.34)$$

where it is assumed that $x_0(k) = -\frac{\hbar k}{eB}$ is the location of the barrier of potential V_{ext} . The first term of $V_{eff}(x)$ is called $V_B(x)$ as it is the contribution induce by the QHE (Figure 2.12 a)).

One can recompute the Landau levels for $\hat{\mathcal{H}}_{eff}$ which depends obviously on k or x_0 :

$$E_n(k) = \hbar|\omega_c| \left(n + \frac{1}{2} \right) + \epsilon_n(k) \quad (2.35)$$

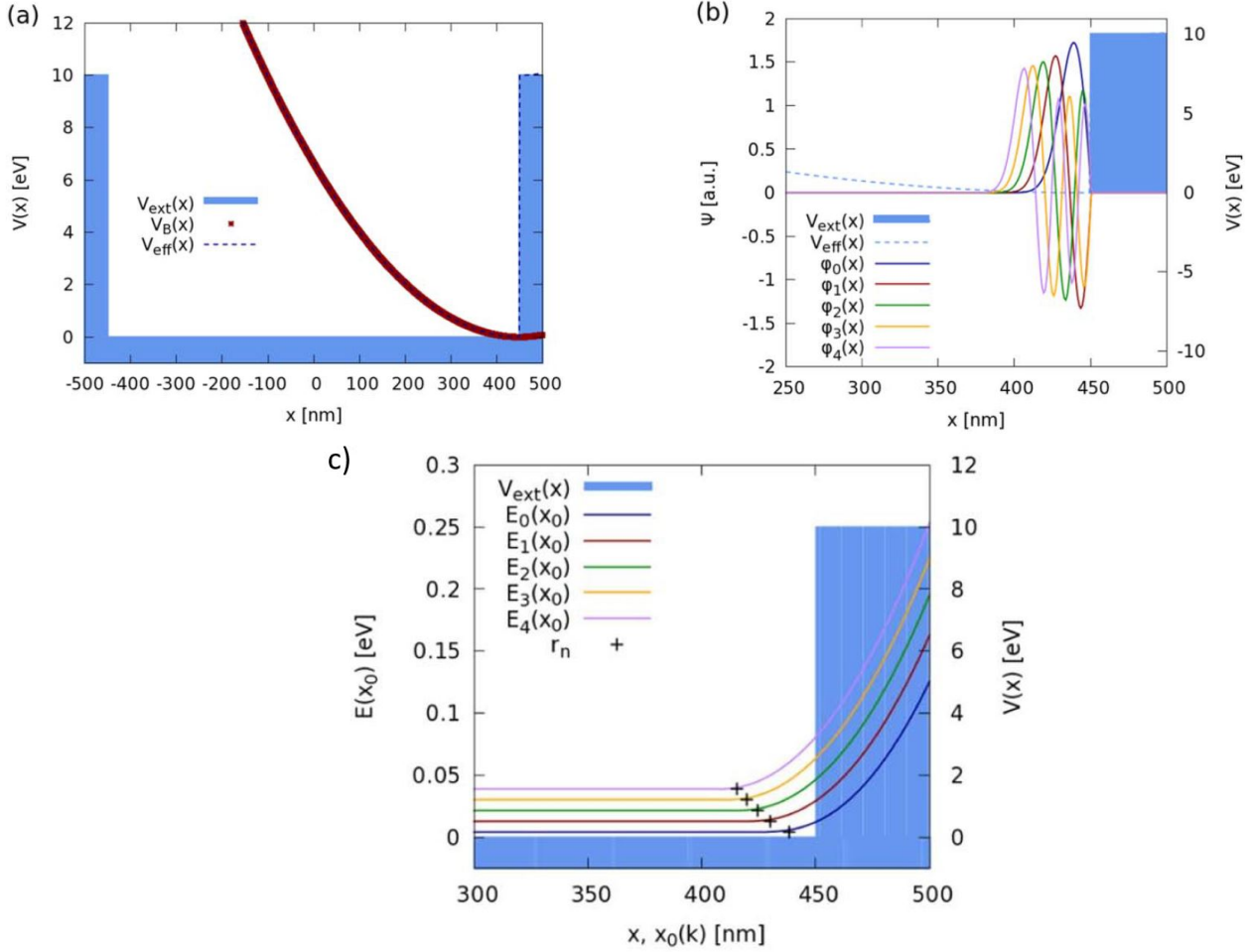


Figure 2.12: (a) Decomposition of the V_{eff} potential in the QHE contribution part V_B and the external potential V_{ext} . (b) ESs $\varphi_n(x, k)$ for $n = [0, 1, 2, 3, 4]$ represented along the x -axis on the right edge with the external potential $V_{ext}(x)$. (c) Landau levels for $n = [0, 1, 2, 3, 4]$ with the abrupt external potential as a function of the x -axis position on one edge. The black crosses indicate the beginning of the interaction with V_{ext} for each n [4].

The first term is equivalent to the one found in the LLs derivation of Equation 2.18. The $\epsilon_n(k)$ term is a correction depending on $V_{ext}(x)$ that tend to bend upward the Landau levels near the edges (Figure 2.12 c)). Far from the barrier, the abrupt external potential is negligible and the Landau levels keep their original shape.

As mentioned previously, an other benefit of working on the ESs is concerning the absence of backscattering. The unidirectional character of the electronic channel is imposed by the chirality of the ESs. To understand it, one use a simpler and a more intuitive classical representation of the sample under perpendicular magnetic field (see Figure 2.13).

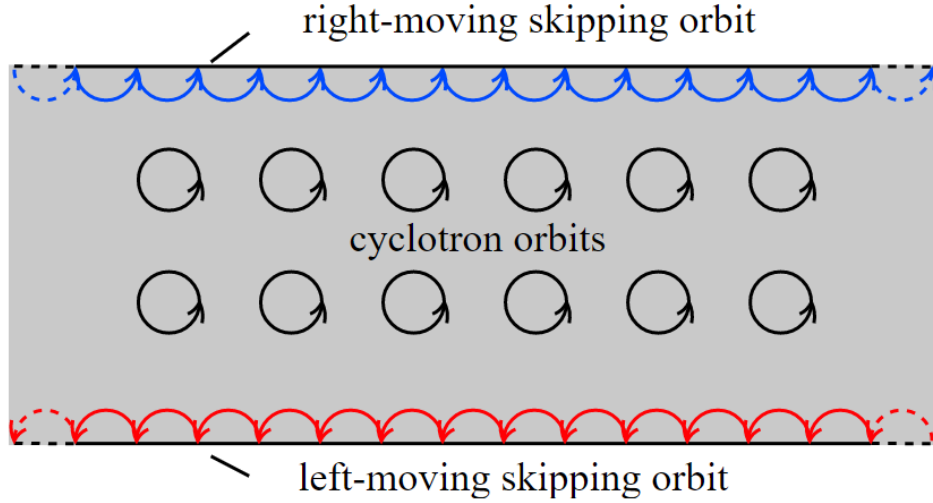


Figure 2.13: Semi-classical representation of the cyclotron and skipping orbits in a sample under magnetic field. The blue and red arrows represents respectively propagating and counter-propagating edge states. The black arrows represents loops of current around defects changing locally the potential [28].

In contrast to cyclotron orbits generated by disorder, charge carriers on the edge are submitted to the Lorentz force that deviate these charge carriers along the limit of the material. The confining potential counterbalances these outwards trajectories and it causes these so-called skipping orbit that propagate without making a closed trajectory. The orientation of B_z determines unequivocally the direction of the ESs. The opposite sides of the sample demonstrates opposite channel direction. Therefore backscattering cannot happen only because it would require charge carriers to move from one side of the sample to the other side. Ballistic transport can be ensured.

Quantum Hall resistivity:

To compute the QH longitudinal and Hall resistivity, it is convenient to write the conductivity tensor [27]:

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ -\sigma_{xy} & \sigma_{xx} \end{pmatrix} \quad (2.36)$$

where σ_{xx} is the longitudinal conductivity and σ_{xy} is the Hall conductivity. By inverting $\boldsymbol{\sigma}$, the conductivity tensor $\boldsymbol{\rho}$ is retrieved:

$$\boldsymbol{\rho} = (\boldsymbol{\sigma})^{-1} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ -\sigma_{xy} & \sigma_{xx} \end{pmatrix}^{-1} \quad (2.37)$$

$$= \frac{1}{\sigma_{xx}^2 + \sigma_{xy}^2} \begin{pmatrix} \sigma_{xx} & -\sigma_{xy} \\ \sigma_{xy} & \sigma_{xx} \end{pmatrix} \quad (2.38)$$

Thus, the Hall and longitudinal resistivity corresponds to:

$$\rho_{xx} = \frac{\sigma_{xx}}{\sigma_{xx}^2 + \sigma_{xy}^2}, \quad \rho_{xy} = \frac{\sigma_{xy}}{\sigma_{xx}^2 + \sigma_{xy}^2} \quad (2.39)$$

When the Fermi level stands between two LLs, the electrical conduction is solely longitudinal through the edge channels. So, $\sigma_{xy} = 0$ which leads to $\rho_{xx} = 0$. However, when the Fermi level stands inside a LL, the electrical conduction is allowed on the entire Hall bar. Thus, the Hall resistivity is finite: $\rho_{xx} \neq 0$.

Concerning the quantum Hall resistance, the classical effect gave $\rho_{xy} = B_z/n_e e$ in Equation 2.6. As each LL is degenerated in two components because of the spins up and down, the filling factor is given by: $\nu = 2n$.

For the relativistic case, the degeneracy of LLs is the two components of spin as well as the two sublattices A and B :

$$\nu = 4\left(n + \frac{1}{2}\right) \quad (2.40)$$

where the second term in the parenthesis is to take into account upper half part of electrons and lower half part of holes in the LL $n = 0$ located at $E = 0$.

Thus, the total electronic density is:

$$n_e = \nu \frac{eB_z}{h} \quad (2.41)$$

By substitution in Equation 2.6, the quantum Hall resistivity is:

$$\rho_{xy} = \frac{h}{\nu e^2} \quad (2.42)$$

Figure 2.14 shows both Hall and longitudinal resistance as a function of the magnetic field. Increasing B shifts the LLs up and intersections with E_F occur. The R_{xy} plateaus are matching the zero R_{xx} .

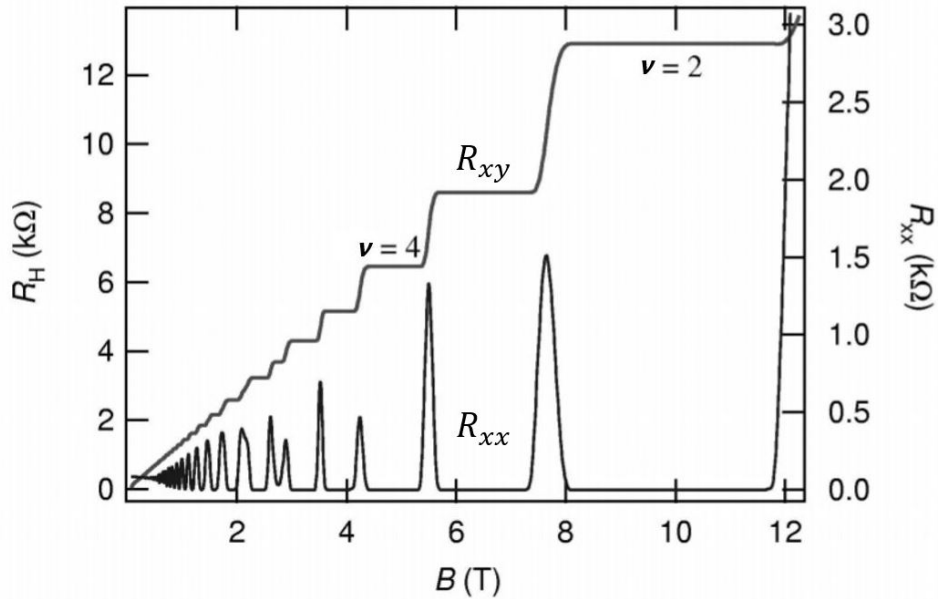


Figure 2.14: Typical R_{xx} and R_{xy} curve as a function of the magnetic field in the QH regime. The upper curves with the plateaus corresponds to R_{xy} and the lower curve with the zeros of resistance corresponds to R_{xx} [29].

2.2.6 Aharonov Bohm effect

The Aharonov Bohm (AB) effect is a remarkable quantum phenomenon in which a vector potential couples with the complex phase of a charge carrier's wave function. That is even more remarkable because, in the original theoretical work [30], the magnetic field creating the phase variation is nonexistent where the charge carriers can move.

Setup:

A small conductor material loop is attached to two arms. Electrons entered the loop on the left arm and divide in two equal amplitudes around the loop. Then, the two electron waves recombine on the right and interfere in the arm. In addition to that, a small solenoid is positioned perpendicular through the loop. The solenoid is supplied in current generating a magnetic field in its center. Thus, the magnetic field is constrained in the solenoid. It means that $\mathbf{B} = \mathbf{0}$ in the wave guide of the loop. However, the vector potential $\mathbf{A}$ is not zero outside the solenoid even if $\mathbf{B}$ and $\mathbf{E} = \mathbf{0}$. In fact, $\mathbf{A}$ is extended everywhere azimuthal to solenoid's axis [31]. A schematic representation is shown on Figure 2.15.

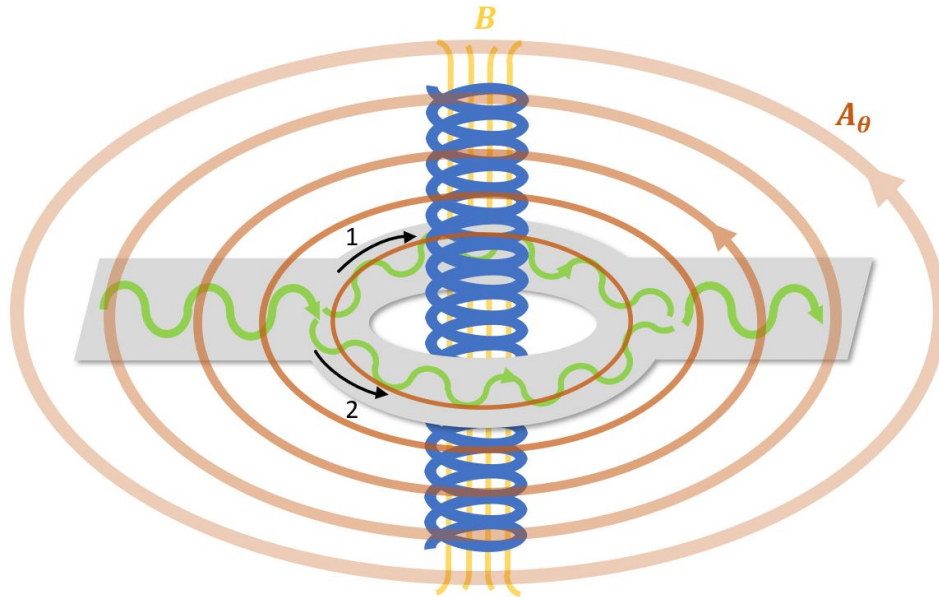


Figure 2.15: Schematic representation of the AB effect in a conductive loop. The electronic wave is split in half while entering the loop: path 1 (from 0 to π) and path 2 (from 0 to $-\pi$). The solenoid creates an enclosed magnetic field B in yellow. The vector potential associated A_θ in brown is spreading outside the solenoid.

Mathematical description:

This mathematical development of this section is inspired by [32].

This vector potential at a radius r can be computed with the help of the Stokes' theorem:

$$\Phi = \int \int \mathbf{B} \cdot d\mathbf{S} = \int \int \nabla \times \mathbf{A} = \oint \mathbf{A} \cdot d\mathbf{l} = 2\pi r A_\theta(r) \quad (2.43)$$

$$\Leftrightarrow A_\theta(r) = \frac{\Phi}{2\pi r} \quad (2.44)$$

where Φ is the magnetic flux generated inside the solenoid.

As developed in Equation 2.9, the momentum of an electron in a magnetic field depends on A . Indeed, the $\mathbf{p}$ term appears in the electronic wave function. So, the energy spectrum of the electron is affected by the flux even if the particle is not in the B field 33. Therefore, the $e\mathbf{A}(\mathbf{r})$ term induce a phase shift between the two electrons path in the loop:

$$\Delta\phi = \frac{1}{\hbar} \left(\int_1 \mathbf{p} \cdot d\mathbf{l} - \int_2 \mathbf{p} \cdot d\mathbf{l} \right) = -\frac{e}{\hbar} \left(\int_1 \mathbf{A} \cdot d\mathbf{l} - \int_2 \mathbf{A} \cdot d\mathbf{l} \right) = \frac{e}{\hbar} \oint_{\text{loop}} \mathbf{A} \cdot d\mathbf{l} \quad (2.45)$$

$$= \frac{e}{\hbar} \Phi \quad (2.46)$$

where $\Delta\phi$ is the phase shift between the two paths.

This expression can be rewritten by introducing the, often used in literature, quantum flux Φ_0 :

$$\Delta\phi = \frac{2\pi\Phi}{\Phi_0} \quad (2.47)$$

where the quantum flux is defined as : $\Phi_0 = h/e$.

For what lies in the following sections, the previous expression is written in term of B and the area it intercepts:

$$\Delta\phi = \frac{2\pi B \Delta A}{\Phi_0} \quad (2.48)$$

These are the two parameters that will be modified to generate patterns of interferences. Figure 2.16 shows R as a function of B . The oscillations are proportional to a squared cosine of the magnetic flux 32 and are the result of alternating constructive and destructive interferences between path 1 and 2.

2.3 Electronic interferometers

Since the first model of matter behaving as a wave has been described by De Broglie, experimentalists have tried to adapt optical interferometers to electrons 34. Originally, with small particles such as electrons. In this manner, Young's double slit experiment, Fabry-Pérot or Mach-Zehnder interferometry had been setup for electrons. The matter waves theory has been proven right. In the following section, Fabry-Pérot interferometers are described first in their classic optical shape. Then, the electronic adaptation is discussed.

2.3.1 Fabry-Pérot

Classical optical interferometer:

Optical Fabry-Pérot (FP) are based on the interferences of multiple transmitted light beams emitted from a single focus source. The generation of many transmitted beams is insured by a cavity composed of parallel partially reflective mirrors. These mirrors are defined by a transmission and reflection coefficient. The interior of the cavity is represented on Figure 2.17 a).

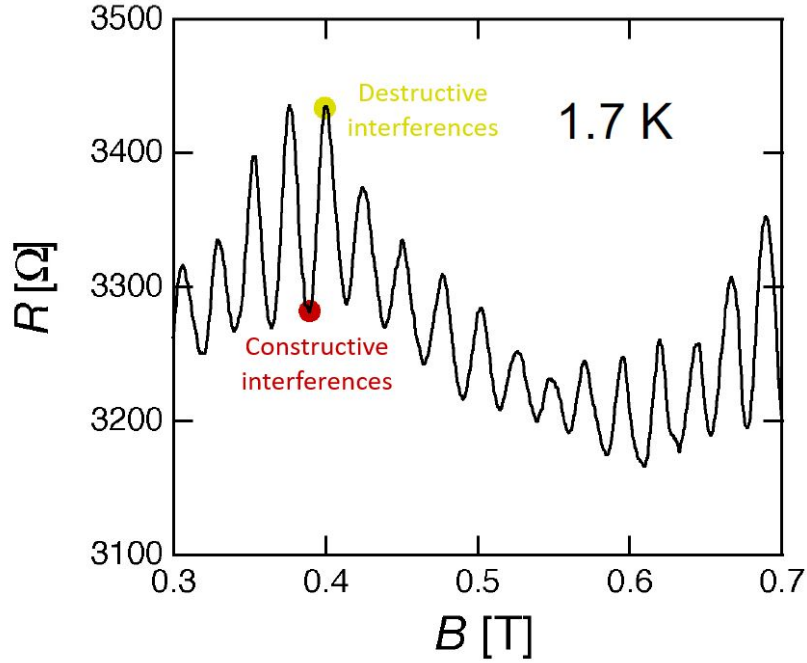


Figure 2.16: Longitudinal resistance as a function the magnetic field demonstrates AB oscillations. The red dot corresponds to constructive interferences at the recombination in the right arm of the loop and the green dot to destructive interferences.

When the incident beam come toward the mirror 1, a part is reflected and the rest is transmitted inside the cavity. The medium for the wave to propagate in the cavity could be different from outside. In this case, the beam is refracted with a specific angle in the cavity (θ on the Figure) . Arriving on mirror 2, the beam is partially refracted and partially reflected inside. These deviations of the beam are repeated until the intensity of the beams become negligible.

The refracted beams are all parallel and directed with the same angle as the incident beam. However, their phase is not the same. These beams had experience different travel length in the cavity depending on the number of reflection before the transmission to the other side. To observe the interferences, a convergent lens is used to focus the refracted beams on a screen. The interference pattern is composed of concentric circles alternating between constructive light spots and destructive dark spots. The phase shift between two consecutive refracted light beams is given by:

$$\Delta\phi = 2knl \cos(\theta) \quad (2.49)$$

where $k = 2\pi/\lambda$ is the wavenumber.

Electronic Fabry-Pérot:

QH regime makes a perfect candidate while trying to convert originally optical interferometers into electronic wave experiments. The reasons behind this are multiple. In 2DEG, ESs are narrow channels with predictable positions and are topologically protected. Their coherence length is notable [7]. They can also be easily deviated by external potentials and make them interact with their counter-propagating channel.

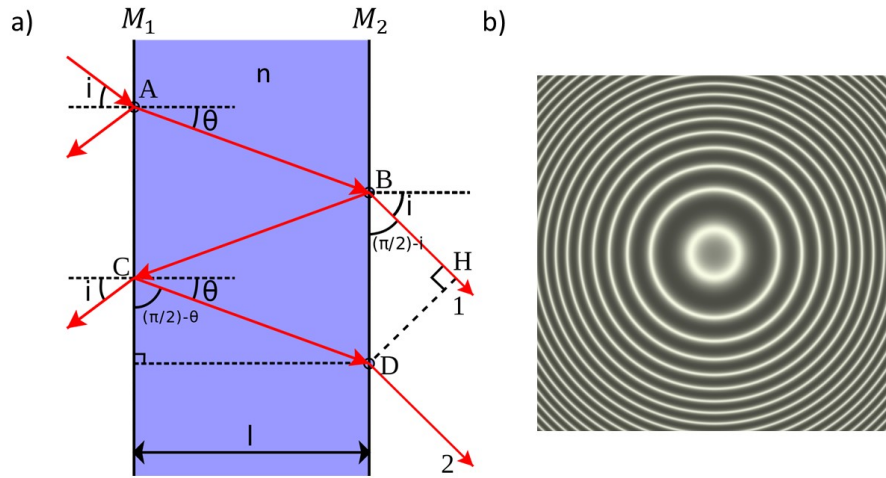


Figure 2.17: (a) Interior of a Fabry-Pérot cavity of length l with a change of the refractive index n . The incident beam is coming with an angle i and is refracted with an angle θ in the cavity. The partially reflective mirrors are labeled with M_1 and M_2 . (b) Typical interferometry pattern associated with the cavity. The light concentric rings corresponds to constructive interferences between the beams refracted by M_2 . The black rings are areas where the beams recombined destructively. Adapted from [35].

In this section, the paper *A tunable Fabry-Pérot quantum Hall interferometer in graphene* by Déprez et al. is briefly reviewed [36].

The starting point of the paper is to construct an electronic interferometer that partition edge channels in the QH regime. These manipulation of ESs have potential application to quantum information processing. [37]

Traditionally, QH FP interferometers experiments have been performed on GaAs heterostructures. Unfortunately, Coulomb blockade effect impedes visibility of the quantum interferences. They decided to switch GaAs semiconductors for graphene which is free of charging effects.

The design of their device is represented on Figure 2.18. The FP cavity is composed of a pair of quantum point contacts (QPCs) with two plunger gates between ¹. In this case, they could get two FB cavity in series. The plunger gates have the purpose of changing the trajectory of the ESs in the cavity and modify the effective interferometer areas. They are polarized with a tension and modify the electrostatic landscape. As a result, the pattern of interference depends on this factor. The Figure 2.19 a) shows the effect of this plunger gate and b) shows the diagonal resistance R_D as a function of the plunger gate voltage V_{pg2} .

Parameters of the simulation:

The back gate voltage is chosen to tune ν_{bulk} in order to have two electron-type edge channels. The QPC₂ and QPC₃ are tuned to reflect totally the inner edge channel while transmitting a portion of the outer channel in the second FP cavity. V_{pg1} is not polarized while V_{pg2} is varied along the experiment, creating oscillations of the diagonal resistance R_D .

¹A QPC corresponds to a constriction of the size of the order of the electronic wavelength, between two conducting areas in the 2DEG. [38]

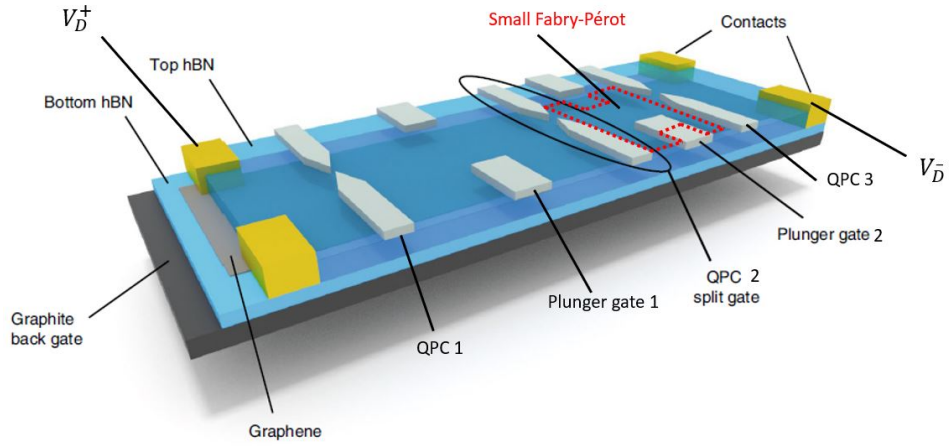


Figure 2.18: Schematic representation of the final device. Graphene is encapsulated between BN layers and this heterostructure is laid on a graphite back gate. On the top BN has been deposited split gates (labeled 1, 2 and 3) and plunger gates (labeled 1 and 2). Contacts have been metallized on each edge of the graphene. The small FP cavity is highlighted in red dotted lines. The transmission of the FP cavities are via the diagonal differential resistance $R_D = d(V_D^+ - V_D^-)/dI$. [36]

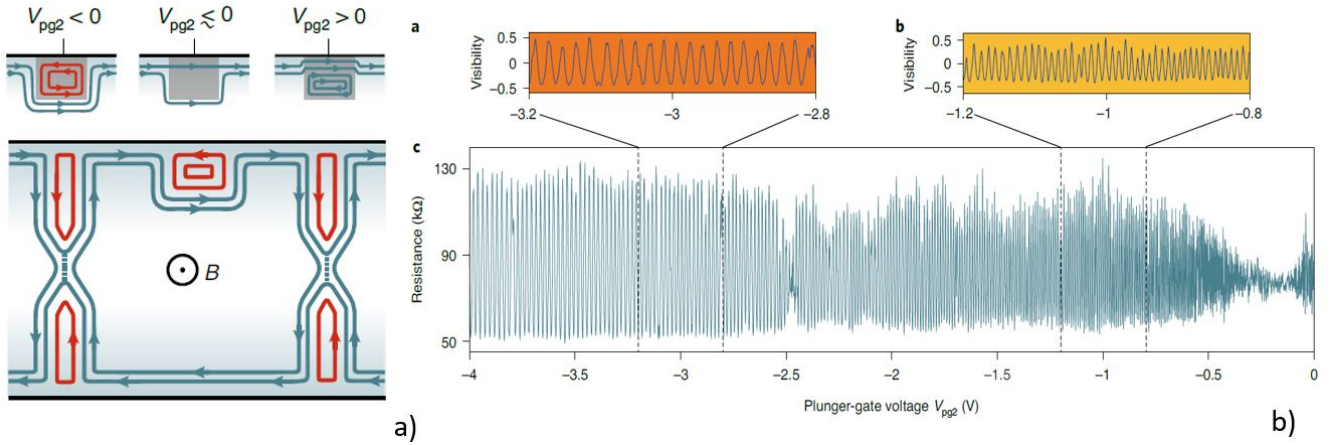


Figure 2.19: (a) Schematic representation of the edge channels in the second cavity. The blue (red) lines indicate electron (hole) carrier channels. The arrows show the direction of propagation. The dashed blue lines at center of the QPCs represent the possibility of tunneling for the electron channels. On top, three different distribution of the channels depending on the value and sign of V_{pg2} . (b) R_D as a function of V_{pg2} . Orange and yellow insets show clear AB oscillations via visibility $(R - \bar{R})/\bar{R}$ graph, where $\bar{R}$ is the average resistance on smaller V_{pg2} ranges.

The second FP cavity configuration of edge channels is represented on Figure 2.19 a). On Figure 2.19 b), the plot of experimental data of R_D as function of V_{pg2} . The insets of this graph allow to highlight FP oscillations for two different ranges of V_{pg2} associated with different configuration of edges channels around the plunger gate.

In conclusion of this paper, high-visibility AB interferences are observed and are in good agreement with theory. It demonstrates that graphene is a great alternative to semiconductors heterostructure while manipulating ESs in a QH FP interferometer.

2.3.2 Scanning gate microscope

Scanning gate microscopes can be a powerful tool to locally gate a chosen region on a conductive device. It takes advantage of the polarized tip of an atomic force microscope (described in further details in Section 4.7) operating at low temperature. The tip is biased with a modular voltage V_{tip} and is scanned above the sample at modular distance d (typically $\sim$ tens of nm). These parameters V_{tip} and d tunes the intensity of the energetic perturbation in the electronic bands and its size in real space. In comparison with scanning tunneling microscope, SGM can access the buried 2DEG in semiconductors.

In particular, the geometry of edge channels in the QH can be modify at will with the perturbation of the SGM tip. On Figure 2.20, a scanning-gate microscopy applied to the imaging of QH electronic transport in buried semiconductor described in the paper *On the imaging of electron transport in semiconductor quantum structures by scanning-gate microscopy: successes and limitations* by H. Sellier, B. Hackens et al. realized partly at UCLouvain.

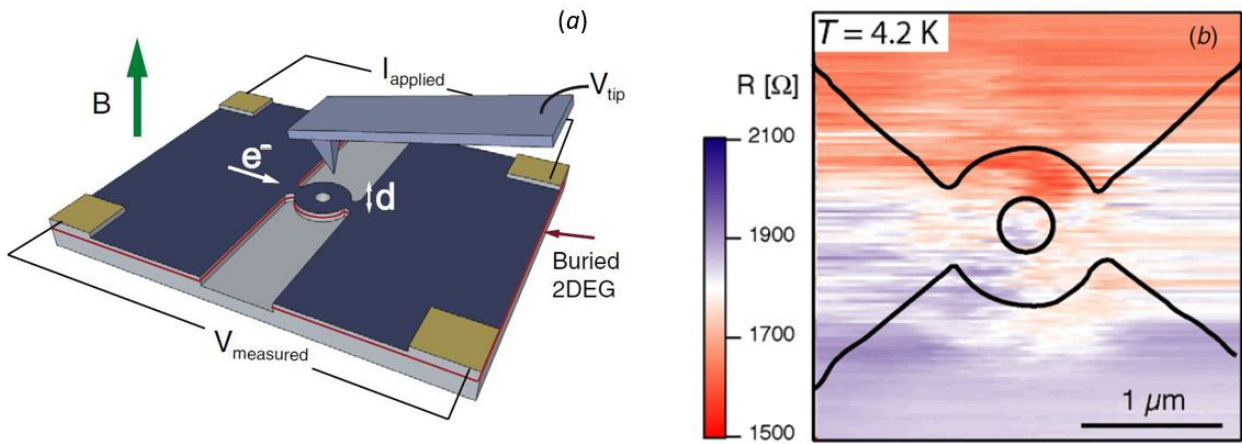


Figure 2.20: (a) SGM applied to a quantum ring. The tip (in light blue) scans the entire ring area with a constant V_{tip} and d . A probe current $I_{applied}$ is applied to the device and measurement of $V_{measured}$ for each tip position allows a 2D resistance mapping of the this quantum ring. (b) Resistance map at $T = 4.2\text{K}$ and $V_{tip} = -1\text{V}$. The black lines represent the quantum ring boundaries.

2.4 InGaAs/InAlAs

First heterostructures were made of semi-conductors and more precisely with GaAs. This section goal is to develop and introduce characteristics for an InGaAs/InAlAs junction [4].

InGaAs and InAlAs are both semiconductors materials forming a heterojunction [39]. Indeed, they have different band gaps. Therefore, the electronic energy bands can be engineered using the right semiconductors. The two materials can be grown by molecular beam epitaxy on InP which is another semiconductor material. This stack of materials forms a VdW heterostructure. Also, doping layers are sandwiched to modulate the electrical properties. A capping layer is often deposited on top of stack. It assists the Ohmic contact formation in the fabrication process [40]. Looking at the band gaps of the junctions (Figure 2.21), a quantum well is formed.

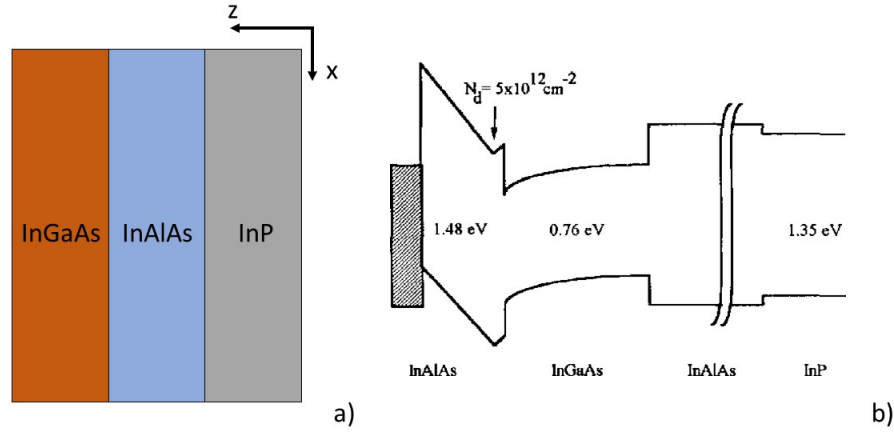


Figure 2.21: (a) Representation of the heterostructure composed of InP substrate and InGaAs/InAlAs on top. (b) Combined energy bands diagram of the stack. Due to the difference in the band gaps, a quantum well is created. The ΔE between the bands are specific for the atomic ratio of InP/InGaAs/InAlAs [41].

When charge carriers are confined in narrow semiconductor quantum well, they behave as a two-dimensional electron gas (2DEG). Thus, the electrons appear to be a 2D plane embedded in a 3D material. The approach developed in section 2.2.3 is still valid in this heterostructure.

A good example of the applicability of heterojunctions for electronic interferometry is the paper *An electronic Mach-Zehnder interferometer* by Y. Ji [42]. The built device was the first equivalent of optical Mach-Zehnder interferometer with electrons. It is based on a 2DEG embedded in a GaAs-AlGaAs heterojunction. AB effect is observed in the QH regime with a single channel split in two paths. QPCs made of biased metallic top gates replace beam splitters and Ohmic contacts are used as detectors (Figure 2.22). The two electronic paths are recombined and interfered in the second QPC.

2.5 Motivation of this work

The goal of this Master Thesis is to explore in a local state how electronic interferometers work in graphene in the QH regime. First, by running simulations using Kwant. Then, by designing, assembling and testing two real devices in laboratory: a single constriction graphene Hall bar and a double constriction graphene Hall bar.

The interferences are created by coupling the propagating channels with the counter-propagating channels. This coupling is allowed thanks to a scanning gate microscope (SGM) tip that modify locally the potential landscape of the graphene. The SGM is a metallic tip allowing to artificially produce a QHI via voltage biased. Creating a QHI with a SGM has already been done on InGaAs/InAlAs junctions allowing to highlight interferences [43]. The interferences are expressed as variation of the resistance due to the AB effect.

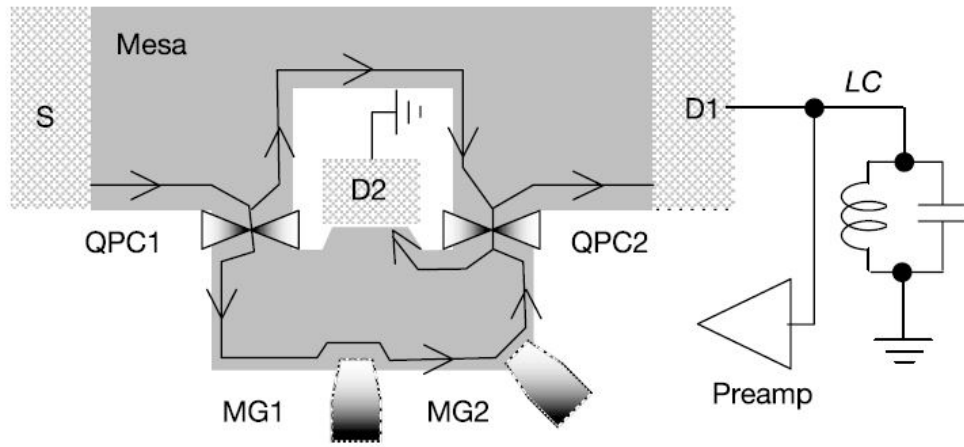


Figure 2.22: Electronic Mach-Zehnder measurement setup. A edge channel is coming towards the first QPC hence splitting the channel in two paths with proportions of electrons depending on the transmission coefficient t_1 of the QPC. Modulations gates MG_1 and MG_2 can tune the length of one a the two paths. These two electronic paths recombine and interfere at QPC2 and are absorbed in D_1 . By varying the voltage of the modulation gates, one of the two paths is modified and AB oscillations appeared. [42].

In the single constriction, the tip is placed in the center of this constriction to create an interferometer. A similar experiment has been already done in [43] but in that case the interferometer is created by a punctual default in the sample and not by an SGM artificially introduced. However, for the second Hall bar, the tip is placed between the two constrictions; which has never been done to this day. This double constriction forms a Fabry-Pérot electronic interferometer and has been studied in [36] but with side gates for the potential perturbation instead of the SGM.

In addition, Section 5 is an analysis of experimental data of S. Faniel that dealt with QHE in a InGaAs/AlGaAs heterostructure. The interferometer is based on a defect creating a natural QHI. Simulations for this experiment on InGaAs/InAlAs are also run in order to compare experimental and simulation results.

Chapter 3

Simulations

3.1 Tight-binding

This section is inspired by [44] and [45].

Exact simulation of physical systems can lead to tremendous calculation times, especially when the number of atoms is increased. In a very small system composed of a few atoms, the actual many-electron wave function can be computed in reasonable times. For larger systems, the computation time is evolving exponentially. Density functional theory (DFT) techniques are used in systems up to thousand of atoms to find the ground state energy of the systems without computing the many-electron wave function. However, to reach mesoscopic and higher scales, tight-binding methods are best tailored. Introduced in 1954 by Slater and Koster, it relies on the calculation of electronic band structure using approximate wave functions [46]. Indeed, the wave functions used in the computation are the same as if the atoms were isolated in their atomic site. The electronic band structure results of the superposition of these wave functions.

3.1.1 Linear combination of atomic orbitals

The true Hamiltonian of a system is written by:

$$H(\mathbf{r}) = H_{\text{at}}(\mathbf{r}) + \sum_{\mathbf{R}_n \neq 0} V(\mathbf{r} - \mathbf{R}_n) = H_{\text{at}}(\mathbf{r}) + \Delta U(\mathbf{r}). \quad (3.1)$$

where H_{at} is the Hamiltonian of a single isolated atom, $V(\mathbf{r} - \mathbf{R}_n)$ is the atomic potential of an atom situated at site $\mathbf{R}_n$ in the lattice and ΔU encodes all the differences between the true potential $H(\mathbf{r})$ and the potential of an isolated atom $H_{\text{at}}(\mathbf{r})$. This corrective term ΔU is approximate by 0 at the center of each atom in the tight-binding theory.

Thus, an electron is not confined in a single atomic orbital $\phi(\mathbf{r})$ but can hop other orbitals as the wave functions are superimposed. The linear combination of these atomic orbitals $\psi(\mathbf{r})$ is given by:

$$\psi_m(\mathbf{r}) = \sum_{\mathbf{R}_n} \alpha_m(\mathbf{R}_n) \phi_m(\mathbf{r} - \mathbf{R}_n) \quad (3.2)$$

where m is the m -th atomic state and α_m is a proportional coefficient.

As for any periodic atomic lattice, this new wave function $\psi(\mathbf{r})$ must obey the Bloch's theorem [47]:

$$\psi(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k} \cdot \mathbf{r}} \psi(\mathbf{r}) \quad (3.3)$$

where $\mathbf{k}$ is the wave vector the electron in the first Brillouin zone. The α_m coefficient can be determined and the wave function becomes:

$$\psi_m(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_n} e^{i\mathbf{k} \cdot \mathbf{R}_n} \phi_m(\mathbf{r} - \mathbf{R}_n) \quad (3.4)$$

Or with *ket* notations:

$$|\psi_m\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_n} e^{i\mathbf{k} \cdot \mathbf{R}_n} |\phi_m\rangle \quad (3.5)$$

where N is the number of lattice sites and the factor $1/\sqrt{N}$ normalize the wave function to satisfy Bloch's theorem.

The energy of the system is computed from the Hamiltonian of the Schrödinger equation:

$$\hat{\mathcal{H}}|\psi\rangle = E|\psi\rangle \quad (3.6)$$

$$\Leftrightarrow E = \langle \psi | \hat{\mathcal{H}} | \psi \rangle \quad (3.7)$$

$$= \frac{1}{N} \sum_m \sum_n e^{i\mathbf{k} \cdot (\mathbf{R}_n - \mathbf{R}_m)} \langle \phi_m | \hat{\mathcal{H}} | \phi_n \rangle \quad (3.8)$$

3.1.2 Calculation of the band structure of graphene

As stated in the section 2.1.2, graphene lattice is decomposed in two sublattices (A and B). Therefore, the wave function $|\psi\rangle$ is the superposition of $|\psi_A\rangle$ and $|\psi_B\rangle$, respectively the wave function of the sublattice A and B:

$$|\psi\rangle = c_A |\psi_A\rangle + c_B |\psi_B\rangle \quad (3.9)$$

From equation 3.7, two expressions are found by applying the bras $\langle \psi_A |$ and $\langle \psi_B |$:

$$\begin{cases} \langle \psi_A | \hat{\mathcal{H}} | \psi \rangle = E \langle \psi_A | \psi \rangle \\ \langle \psi_B | \hat{\mathcal{H}} | \psi \rangle = E \langle \psi_B | \psi \rangle \end{cases} \quad (3.10)$$

$|\psi\rangle$ is replaced by its expression in equation 3.1.2 and the system is expressed as a single matrix:

$$\begin{pmatrix} \langle \psi_A | \hat{\mathcal{H}} | \psi_A \rangle & \langle \psi_A | \hat{\mathcal{H}} | \psi_B \rangle \\ \langle \psi_B | \hat{\mathcal{H}} | \psi_A \rangle & \langle \psi_B | \hat{\mathcal{H}} | \psi_B \rangle \end{pmatrix} \cdot \begin{pmatrix} c_A \\ c_B \end{pmatrix} = E \begin{pmatrix} c_A \\ c_B \end{pmatrix} \quad (3.11)$$

where $\langle \psi_A | \psi_B \rangle = \langle \psi_B | \psi_A \rangle = 0$ because wave functions decay rapidly away from $\mathbf{r} = 0$, meaning that the overlap is considered equal to 0 and $\langle \psi_A | \psi_A \rangle = \langle \psi_B | \psi_B \rangle = 1$ because it corresponds to the same atomic site.

For simplicity, $\langle \psi_X | \hat{\mathcal{H}} | \psi_Y \rangle$ is rewrite as E_{XY} . Both sublattices are symmetric by translation, thus:

$$E_{AA} = E_{BB} \quad (3.12)$$

$$E_{AB} = E_{BA}^* \quad (3.13)$$

Eigenvalues computed from equation 3.1.2 are given by:

$$E_{\pm} = E_{AA} \pm |E_{AB}| \quad (3.14)$$

The two terms of $E_{\pm}$ can be developed with the help of the Bloch's theorem:

$$E_{AA} = \frac{1}{N} \sum_n \sum_m e^{i\mathbf{k} \cdot (\mathbf{R}_{A,n} - \mathbf{R}_{A,m})} \langle \phi_{A,m} | \hat{\mathcal{H}} | \phi_{A,n} \rangle \quad (3.15)$$

$$E_{AB} = \frac{1}{N} \sum_n \sum_m e^{i\mathbf{k} \cdot (\mathbf{R}_{A,n} - \mathbf{R}_{B,m})} \langle \phi_{B,m} | \hat{\mathcal{H}} | \phi_{A,n} \rangle \quad (3.16)$$

Only the nearest neighbors of an atom are considered. Specifically, nearest neighbors of an atom in sublattice A (B) are three atoms in sublattice B (A). Therefore, expressions 3.15 and 3.16 can be simplified:

- E_{AA} term: $\mathbf{R}_{A,n} - \mathbf{R}_{A,m} = 0$ is the only existing one. That is the on-site energy term noted E_0 . For simplicity, E_0 is set à 0.
- E_{AB} term: $\mathbf{R}_{A,n} - \mathbf{R}_{B,m} = \delta_1, \delta_2$ or δ_3 . With the hopping parameter t defined as: $t = \langle \phi_{B,m} | \hat{\mathcal{H}} | \phi_{A,n} \rangle$, one can derive the expression:

$$|E_{AB}| = \pm t \sqrt{1 + 4 \cos^2(\sqrt{3}k_x a) + 4 \cos\left(\frac{\sqrt{3}}{2}k_x a\right) \cos\left(\frac{3}{2}k_y a\right)} \quad (3.17)$$

Finally, the expression 3.17 can be developed in Taylor series near the points $\mathbf{k} = K_+ + \delta\mathbf{k}$ and $\mathbf{k} = K_- + \delta\mathbf{k}$ that corresponds to the confluence of the conduction and valence bands 48:

$$E_{\pm}(\mathbf{k}) \approx \pm \hbar v_F |\mathbf{k}| \quad (3.18)$$

3.2 Kwant package

The simulation process is a critical part of the physical understanding. This chapter is focused on the simulation of two different sample geometries described below.

Kwant is a powerful free python package allowing numerical calculations and tight-binding models with a strong focus on quantum transport. The advantages of Kwant is its flexibility and the ease of use.

A vast variety of system and quantum phenomena can be simulated with Kwant. The following examples are based on the Kwant open source documentation 49:

- Figure 3.1: Graphene flake crystal structure with its wave function of low energy eigenstate represented by blue disks.
- Figure 3.2 and 3.3: Quantum Hall effect. On the right, the graph clearly shows the QHE with the quantization of the conductance represented by the apparition of plateaus.

All these examples shows that Kwant is able to simulate lot of different physical systems. It is definitively a complete and reliable package allowing to simulate a graphene Hall bar and to highlight electronic interferences.

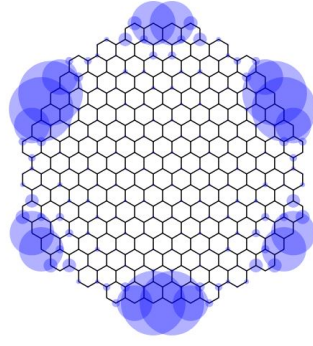


Figure 3.1: Graphene flake.

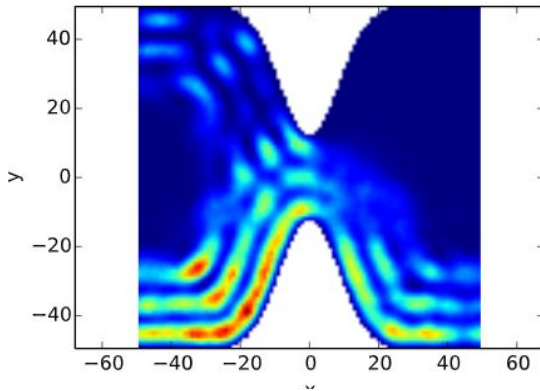


Figure 3.2: Conductance through a 2-d electron gas.

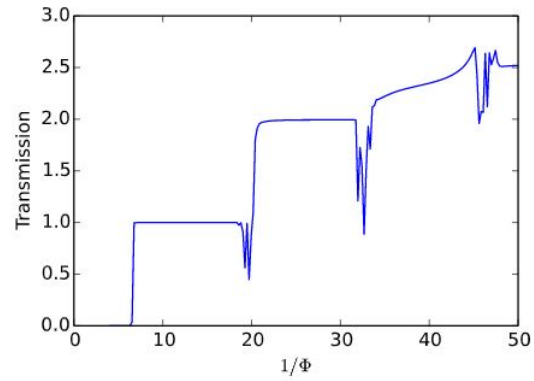


Figure 3.3: Transmission as a function of magnetic flux in a 2DEG.

3.3 General considerations

Reading published papers concerning electronic interferometry in the QHE have been inspirational to define the kind of geometry and the type of interferences sought in this work. Notably, *Upstream modes and antidots poison graphene quantum Hall effect* by N. Moreau et al. and *A tunable Fabry-Pérot quantum Hall interferometer in graphene* by C. Deprez et al. Based on these, the decision has been taken to simulate and build in laboratory two different geometries: a graphene Hall bar with a single constriction located at mid-length and a graphene Hall bar two constrictions next to each other at the center of the bar. These two designs lead to two different experiments but in both cases, a SGM tip is used to vary locally the electrostatic landscape. In the single constriction, the tip is placed between the two apex of the constriction and act like a QPC. In the double constriction, the tip is place on the edge of the sample to modify the electronic path between the two constrictions.

3.4 Single constriction

The Figure [3.5](#) shows the single constriction Hall bar design described in the previous section. For the simulations, a length of $1 \mu\text{m}$ and width of $0.5 \mu\text{m}$ has been chosen. The indentation depth is 125 nm and the constriction aperture is 250 nm. The transverse resistance R_{xx} is measured between

leads on both sides of the constriction:

$$R_{xx} = \frac{dV_{xx}}{dI} \quad (3.19)$$

It is behind this parameter that interferences are hidden.

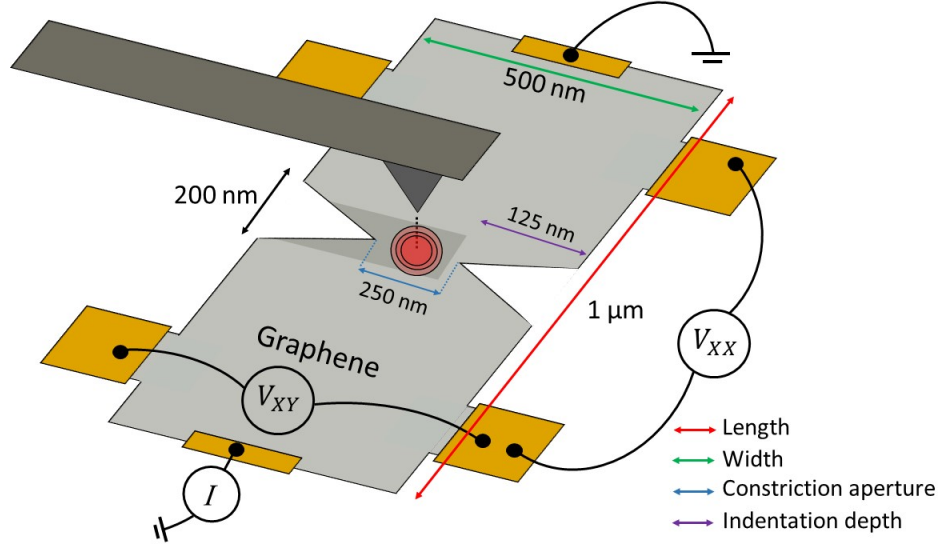


Figure 3.4: Schematic view of the single constriction with the SGM tip potential centered between the two apex of the constriction.

Thanks to the coupling between edge channels and the applied potential, current can flow from one side to the other side of the Hall bar (Figure 3.5 and 3.6). Charge carriers trapped around the quantum island interferes with themselves. AB oscillations can be achieved by varying the strength of the magnetic field or by varying the flux quantum ϕ .

3.4.1 Simulation parameters

- Magnetic field $B = 8$ T: These magnitudes of magnetic field are achievable in laboratories. Moreover, LL energy E_n is proportional to the square root of B . So, choosing a high value of magnetic field will push apart the energy levels. Thus, there is more room to select a precise LL. However, with 8 T the LL are not shifted to unreasonable energies. Interceptions with the Fermi level are still available in the linear dispersing Dirac cone. Overall, this range of value for the magnetic field is often used in literature for this kind of experiment.
- Tip potential amplitude $E_{tip} = 0.05$ eV: It corresponds to the variation of energy in the graphene electronic bands linked to the tip potential V_{tip} . This value is set quite low for two reasons. First, dealing with a small bump of potential allows only one or a few intersections between E_F and LLs. It is useful to facilitate interpretation of the simulations because only one edge channel can simultaneously tunnel via the QHI. The other reason is linked to quite large thickness of the exfoliated BN in laboratory. Indeed, it is about ~ 100 nm thick. Therefore, the SGM tip cannot be very close to the graphene and the potential induced is weak.
- Scaling parameter $s = 8$: The scaling parameter is a trick to reduce the number of atoms in the system while keeping the desired sample dimensions. The simulation running time is largely

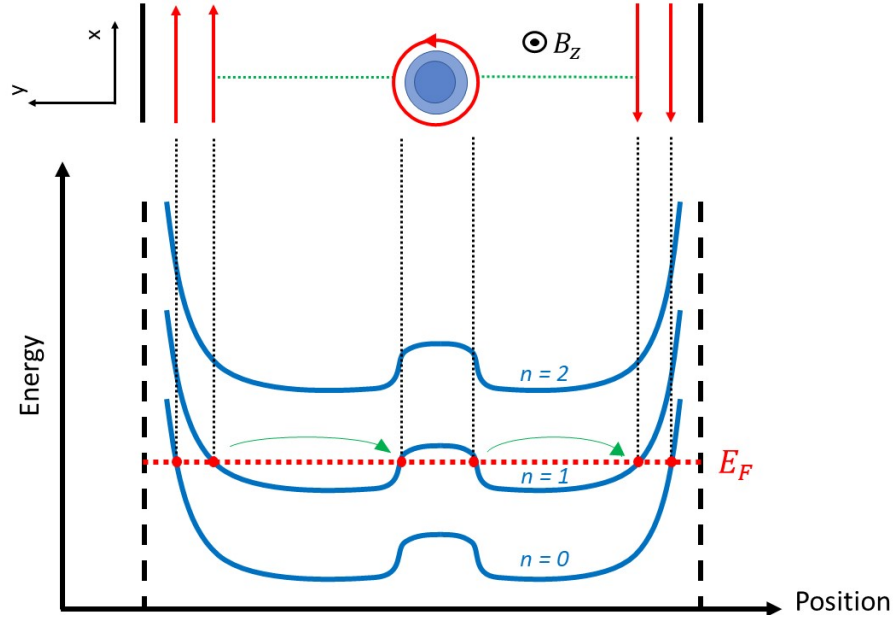


Figure 3.5: Edge channels (blue continuous lines) from $n = 0$ to 2 with a central tip potential. Intersection between a Landau level and the Fermi energy (red dotted line) create a channel. Charge carriers have the possibilities in proper condition to tunnel from the edge to the quantum island (green dotted lines).

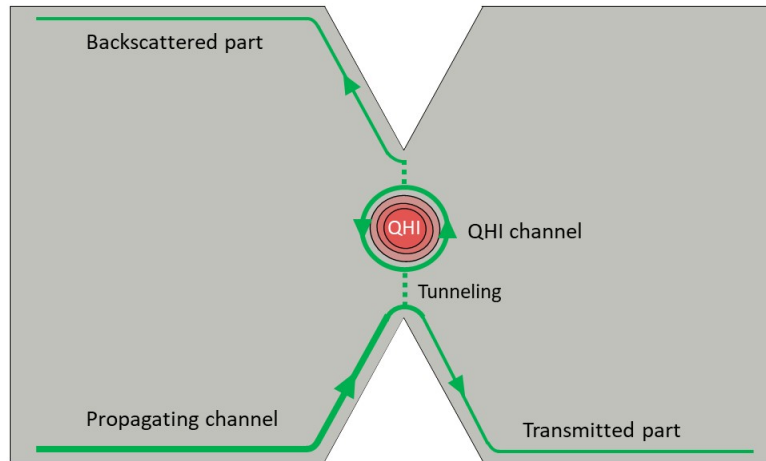


Figure 3.6: General view of an edge channel in the single constriction with the tip potential. A part of the charge carriers in the ES is transmitted through the QPC and another part is backscattered by tunneling via the QHI.

reduced and the quality of results is still decent while s is not too high. The value of 8 has been a good agreement between running time and quality results.

- Fermi energy $E_F = 0.175$ eV: With the previous value of magnetic field and scaling parameter,

the maximum value of the Fermi energy to stay in the linear regime of graphene is 0.175 eV.

$$E_{f,max} = \frac{t}{2} \quad (3.20)$$

with t the hopping parameter $t = \frac{2.8}{s}$.

With these parameters combined, the energy levels across the length of the sample are given on Figure 3.7. It corresponds to a $N/N'/N$ junction with respective filling factors 6/2/6. The LL interacting with the tip potential is $n = 1$.

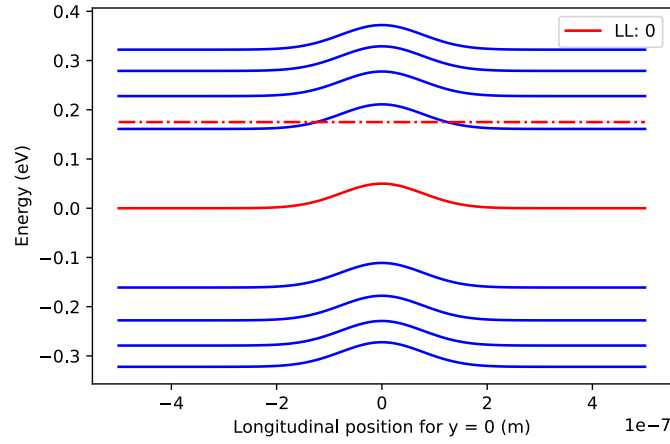


Figure 3.7: Energy of the Landau levels with the chosen parameters. It is a cross-section along the length of the Hall bar.

3.4.2 Generation of interferences

As reviewed in the State of the Art, the Aharonov-Bohm effect is detected when the number of flux quanta passing through the current loop is varying. In this case, the loop is generated by the tip potential crossing the Fermi level. Resistive oscillations come from destructive interferences when ϕ is a multiple of ϕ_0 and destructive halfway between.

Thus, there are two ways to generate theses AB interferences:

- Varying the potential width: Increasing the size of the tip potential allow more quantum flux to intercept the interior of the quantum island.
- Varying the magnetic field magnitude: Increasing B will increase the quantum flux density and therefore varying the number of flux quanta passing through the loop. Moreover, increasing B shifts the LL to higher energies. It means that the intersection of the tip potential with the constant Fermi level will be shifted down. The surface of the quantum island is larger.

This energy shift is represented on Figure 3.8

Concerning the potential, it is generated in laboratory with a SGM polarized tip. To be as realistic as possible, the potential is not defined as a sharp step but a Lorentzian [50]. For the sake of simplicity, the Lorentzian is substituted by a 3D Gaussian function given by the following formula:

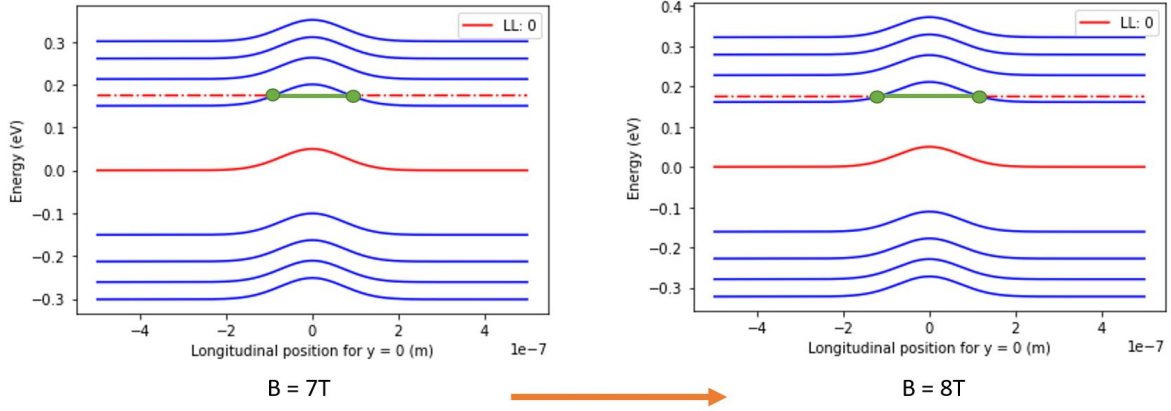


Figure 3.8: Evolution of the Landau levels energy with the magnetic field and a constant Fermi level. For instance, LL $n = 1$ at $B = 7$ T is standing at ~ 0.15 eV while at $B = 8$ T LL $n = 1$ is at ~ 0.17 eV. The intercept Fermi level with the LL $n = 1$ is highlighted in green.

$$V_{tip} = A \cdot \exp \left(- \left(\frac{(x - x_0)^2}{2\sigma_x^2} + \frac{(y - y_0)^2}{2\sigma_y^2} \right) \right) \quad (3.21)$$

with A the amplitude, (x_0, y_0) the center of the tip potential and (σ_x, σ_y) the standard deviation. Three parameters can be changed, the position, the width and the amplitude of the potential.

3.4.3 Evolution of the longitudinal resistance with the potential width

The first simulation is focused on the potential width by changing the standard deviation as shown on the diagrams of Figure 3.9.

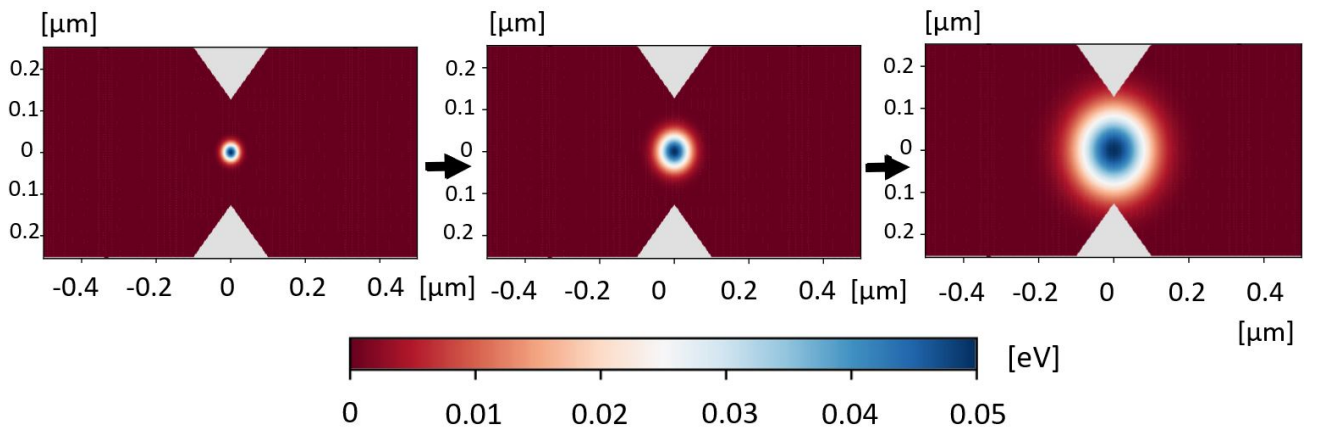


Figure 3.9: Schematic representation of the first simulation. The potential tip spreads across the constriction while keeping the amplitude of the Gaussian constant.

The longitudinal resistance according to the potential width is represented on Figure 3.10. A quick look at this graph bring out straight three pieces of information: the resistance is globally increasing,

there are periodic sinusoidal oscillations and those oscillations shift in amplitude along the curve. These effects are detailed in the following:

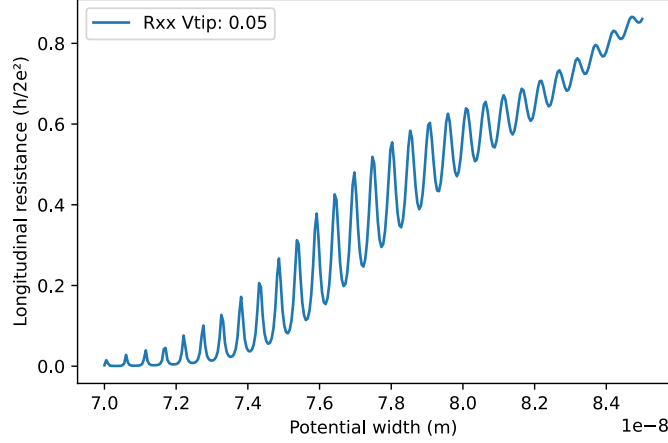


Figure 3.10: R_{xx} as a function the potential width for the simple constriction.

- The global increase can be seen as a variation of the reflection/transmission coefficient of the constriction. By analogy, without potential and reducing the spacing between the two apex of the constriction will lower the transmission of the charge carriers through this constriction. A bigger portion of current is deflected and backscattered on the other edge of the graphene. This is similar in some ways with this experiment. Indeed, increasing the potential width will bring closer the edge channel with the QHI. The coupling between these two become more intense. A part of the electrons is still transmitted through the gate but some tunnel to their QHI channel. The sample being symmetric, those electrons can also tunnel from their QHI channel to the other edge of the graphene in the counter-propagating channel. Overall, R_{xx} increases with the potential width as more carriers are backscattered to the counter-propagating edge. On Figure [3.11](#), here is an example of the current density map along the graphene. The propagating channel is flowing from down left to down right of the sample. At the apex of the constriction, part of the current is transmitted and part of it is encircling the potential. The heat map also shows a slight current density backscattered on the top counter-propagating edge.
- Secondly, the constant frequency sinusoidal oscillations are the signature of a channel interfering around the QHI. Those patterns were assigned to AB oscillations. To verify this assumption, let's check with the formula linking the phase shift with the variation of the area intercepted by the magnetic field from Equation [2.48](#):

$$\Delta\phi = \frac{2\pi B \Delta A}{\phi_0} \quad (3.22)$$

In this case, ΔA is the disk obtained by the interception between the Fermi energy and the tip potential.

Theoretically, the phase shift between two minima is: $\Delta\phi = 2\pi$. Using equation [3.22](#), $\Delta\phi$ can be computed with the variation of A of the simulation data. The phase shift found is:

$\Delta\phi = 0.956 \cdot 2\pi$. This value is close enough from 2π to confirm that these high frequency oscillations are caused by AB effect.

- Finally, concerning the variation of the amplitude of the modulated sinusoid. Figure 3.12 brings a short qualitative model separated in three parts.

The *a)* panel corresponds to the regime of low amplitude oscillations in the beginning of the curve in Figure 3.10, panel *b)* corresponds to the large amplitude oscillations located mid-curve and panel *c)* are the lower amplitude oscillations at the end of the curve.

In panel *a)*, the coupling between the edge channel and the QHI is weak. The probability of tunneling for electrons is low. With only a small part of the current, the magnitude of the AB oscillations is limited. It increases with the coupling and the bigger surface of the QHI. In panel *b)*, the probability to tunnel in the channel around the QHI is high. The sinusoid has maximal amplitude until it enters the regime of panel *c)* and starts decreasing. In fact, almost the entire channel is deviated around the QHI. However, when the potential size becomes too large and starts overlapping the constriction, most of the propagating channel cannot make a full loop. It is deviated directly to the counter-propagating top edge. The amount of charge carriers looping around the QHI is not that big anymore. The magnitude of the AB oscillations starts to decrease. The difference of amplitude between minima and maxima is highlighted on Figure 3.13.

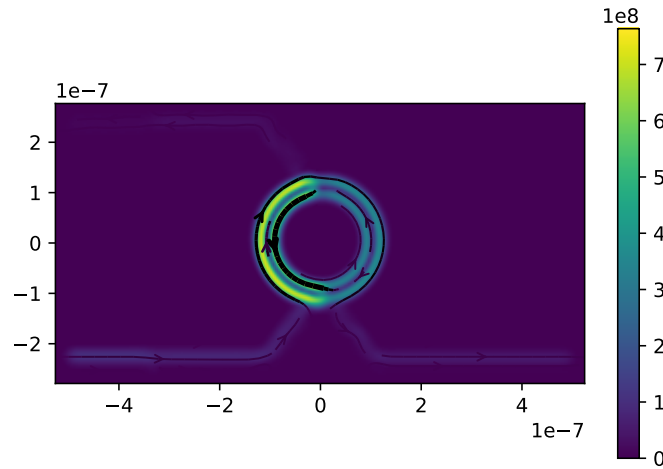


Figure 3.11: Heat map of the current density for the sample.

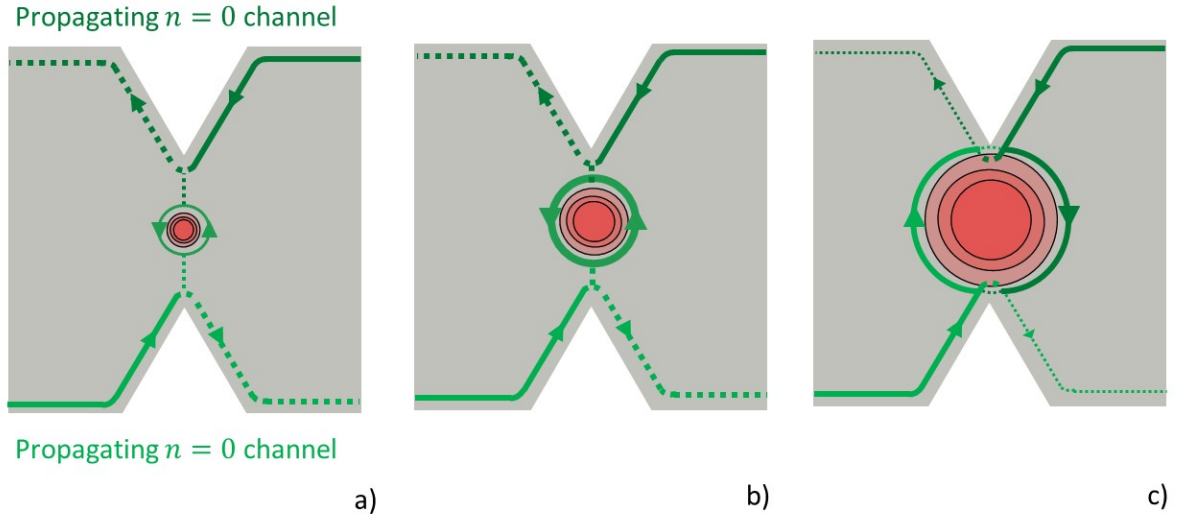


Figure 3.12: Evolution of the trajectories of the edge channel $n = 0$ for a growing tip potential. The thickness of the green loop around the potential indicates the amount of electrons available to interfere.

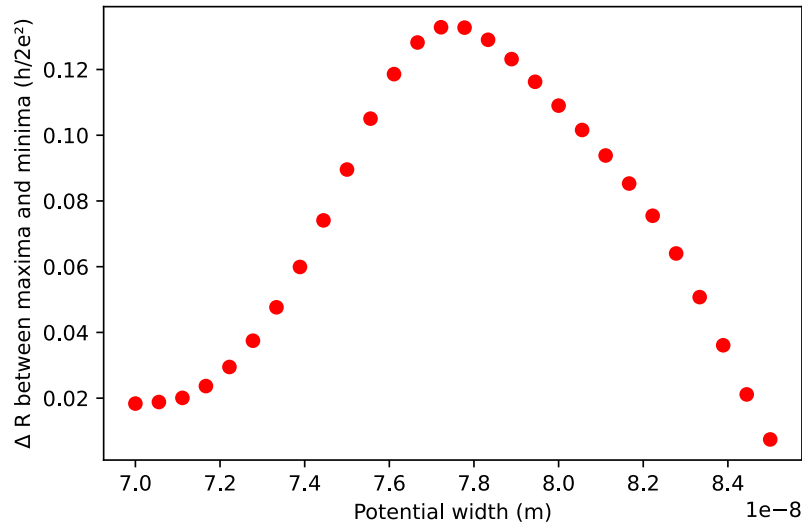


Figure 3.13: Variation of the resistance amplitude between maxima and minima next to each other along the increase of the potential width.

3.4.4 Comparison for different tip positions on the y -axis.

During the experimental process, it would be quite tricky to exactly center the tip of the SGM in-between the constriction. For this reason, simulations of potential slightly shifted horizontally or

vertically have been explored. Figure 3.14 highlights three different positions along the transverse axis.

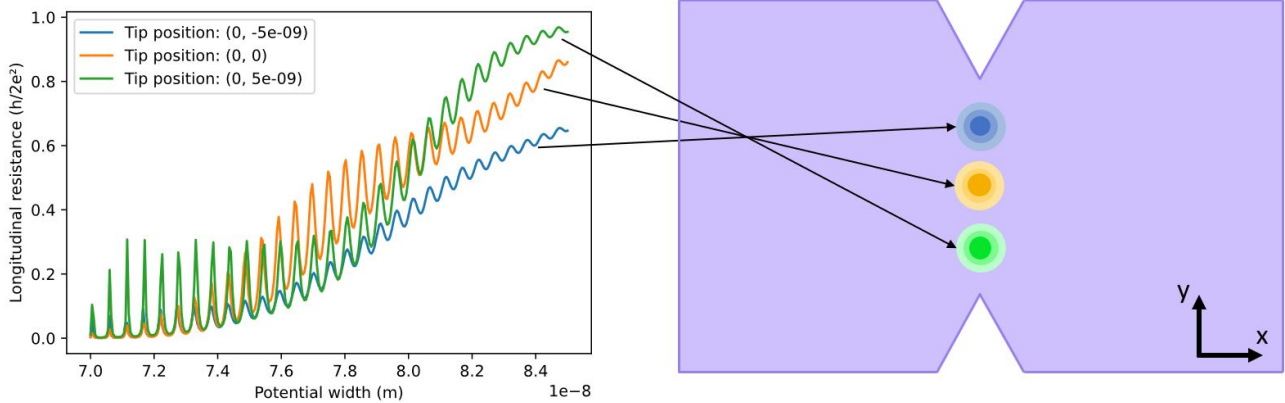


Figure 3.14: Longitudinal resistance for different tip positions on the y -axis. The green curve corresponds to the tip shifted down by 5 nm, the orange one is centered and the blue one corresponds to the tip shifted up by 5 nm.

From this graph, several observations are easily made. First, different position of the tip lead to different global longitudinal resistances (1). Then, the green curve shows resistive peaks from the beginning whereas the blue and orange curves start oscillating around $7.4 \cdot 10^{-8} \text{m}$ (2). Finally, from a certain potential width, the curves are no longer synchronized (3). These observations are respectively explained with the following assumptions. Before doing that, one needs to specify that R_{xx} is computed on the top edge of the sample.

1. The green corresponds to the tip potential closest to the top constriction. It means that the coupling between the QHI and the edge channel is the most intense in comparison with the two other curves. Probabilistically, there are more carriers at stake around the QHI with the green potential. Those have the possibility to backscatter on the other edge, which account for a global higher resistance. Inevitably, the blue curve corresponds to the furthest QHI from the constriction.
2. The greater coupling for the green curve induces the regime of AB oscillations starting sooner/stronger than the others.
3. A priori, the curves should stay synchronous with each other as the potential width is increasing at the same rate in the three cases. It is the truth and the curves oscillate in phase up to potential width of about 75 nm ¹. This corresponds to the moment where the QHI starts to overlap the constriction. While the QHI is growing, there is a part of the island that is not filled with graphene. Because, the orange and blue potentials do not overlap the constriction at the same time, they loose their synchronization. Figure 3.15 can help to visualize the situation.

One can verify the short model introduced in section 3.4.4 for the green and blue curve:

¹As a reminder, the radius of the QHI is not exactly equal to the potential width. What is called potential width is in fact the width at mid-height of the Gaussian. With the flattened Gaussian used in this work, the area of the QHI is larger than the area associated with the potential width.

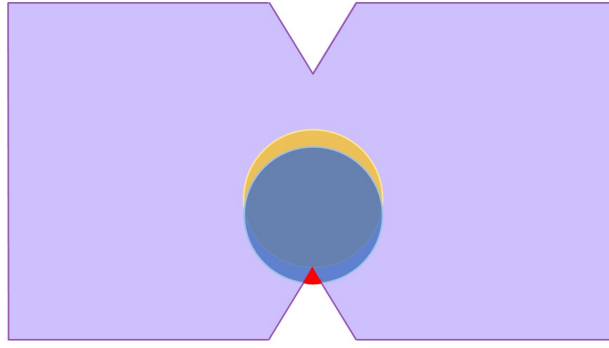


Figure 3.15: Positioning of the blue and orange tip potential close to the constriction apex. Because the one is shifted down in comparison to the other, the blue one will overlap the constriction first while the orange one is still fully on graphene. The red pie shaped area does not account for the intercepted magnetic flux of the blue potential.

- Green curve: oscillations start strong as the potential is shifted from the beginning to the top edge while progressively mitigate from 75 nm potential width. In this second part, the potential is too close from the constriction to allow a full loop of current to flow around the QHI (panel c) of Figure 3.12).
- Blue curve: As it is shifted down, the coupling with the potential is practically nonexistent in the beginning. Then, two effects annihilate themselves to generate quasi constant resistance peaks. The coupling is becoming more intense bringing a positive component to the peaks. Meanwhile, current loop around the QHI are not full because of the proximity with the down constriction. Therefore, it mitigates the amplitude of the oscillations.

3.4.5 Comparison for different tip positions on the x -axis

The graph on Figure 3.16 shows 3 different curves associated to three different positioning of the potential tip along the longitudinal axis. It reveals that the global resistance decreases when the tip is moving from the left to the right of the constriction. It is a surprising result. Indeed, the coupling should be the same from the constriction to the blue potential and from the constriction to the green potential. These variations of resistance cannot be explained at the moment.

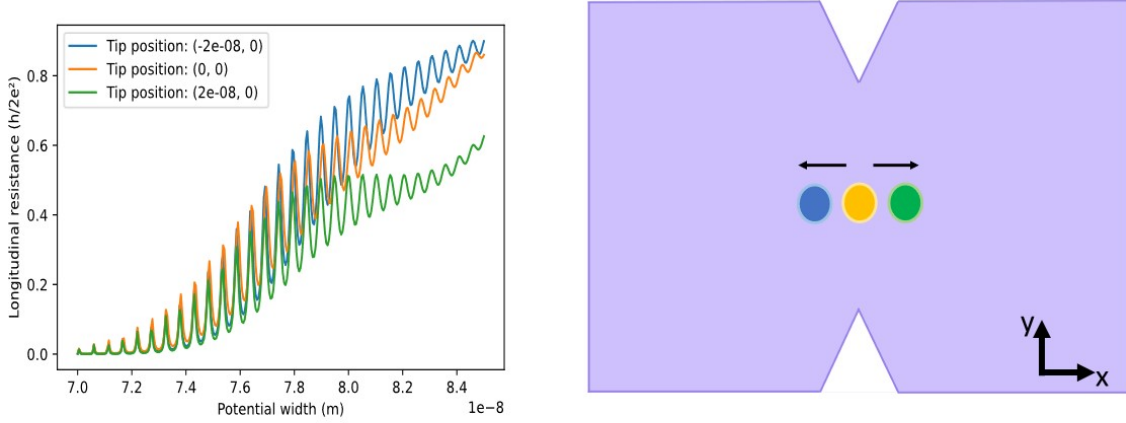


Figure 3.16: Longitudinal resistance for different tip positions on the x -axis. The blue curve is shifted to the left by 20 nm, the orange one is centered and the green one is shifted to the right by 20 nm.

3.4.6 Evolution of the longitudinal resistance with the magnetic field

As described in the section 3.4.2, another way to highlight interferences is to modify the magnetic field while keeping the potential width constant. The Figure 3.17 shows R_{xx} for a range of $B = [7.5; 8.3]$ T. In addition to the greater density of the quantum flux intercepted, the variation of the QHI area is shown on Figure 3.8 as the magnetic field is increased, Landau levels are moving upwards with respect to the Fermi energy, which enlarges the area of the QHI. Indeed, in graphene, the LL energies are expressed as [51]:

$$E_n = \pm v_f \sqrt{2\hbar e} \sqrt{n B_z} \quad (3.23)$$

The LL energies are proportional to the square root of the magnetic field.

Concerning the behavior of the graph, the curve follows the same pattern as the simulation of section 3.4.3. As expected, increasing B leads to electronic backscattering on the counter-propagating edge channel. It is accompanied by the high frequency AB oscillations between two maxima for every new magnetic quantum flux intercepted in the QHI.

3.4.7 Fabry-Pérot quantum model

One can compare the single constriction device to a FP interferometer. Indeed it has similar components and more precisely two QPCs having a transmission and reflection coefficients. For a FP interferometer, the transmission probability function can be expressed like the following:

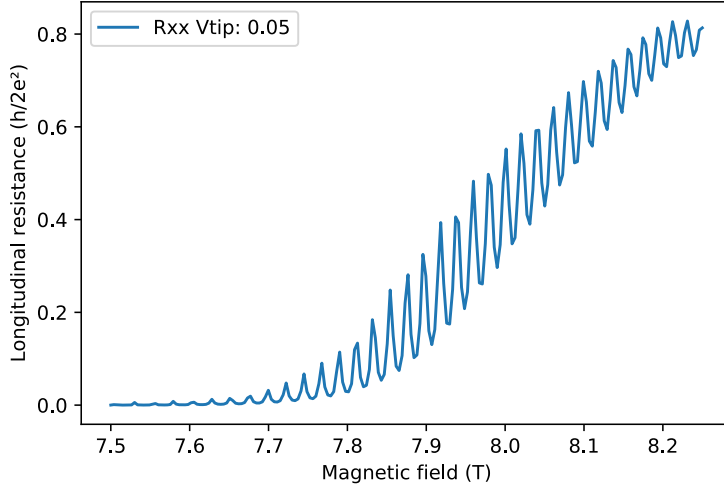


Figure 3.17: Longitudinal resistance as a function of the magnetic field magnitude for the simple constriction.

$$T(\epsilon, \Phi) = \frac{|t_1|^2 |t_2|^2}{1 + |r_1 r_2|^2 - 2|r_1 r_2| \cos(2\pi \frac{\Phi}{\Phi_0} + \frac{2L\epsilon}{\hbar v} + \phi)} \quad (3.24)$$

with t_1 and t_2 the transmission parameters, r_1 and r_2 the reflection parameters which can be expressed as $1 - t_1$ and $1 - t_2$, $2\pi \frac{\Phi}{\Phi_0}$ the Aharonov-Bohm phase, $\frac{2L\epsilon}{\hbar v}$ the dynamical phase and ϕ a constant phase factor.

By analogy in the single constriction device, the transmission t_1 is between the propagating edge channel and the tip potential (QPC₁) and the transmission t_2 between the tip potential and the counter-propagating edge channel (QPC₂) (see Figure 3.18). These coefficients are governed by the width and the position of the potential. If the tip is placed at the center, QPCs coefficients are the same by symmetry. On the contrary, if the tip is shifted up or down in comparison with the device center, coefficients will not be equal anymore.

It is possible to express Equation 3.24 only with transmission coefficients of both cavities knowing that $r_1 = 1 - t_1$ and $r_2 = 1 - t_2$. In that case, Equation 3.24 becomes:

$$T(\epsilon, \Phi) = \frac{|t_1|^2 |t_2|^2}{1 + |(1 - t_1)(1 - t_2)|^2 - 2|(1 - t_1)(1 - t_2)| \cos(2\pi \frac{\Phi}{\Phi_0} + \frac{2L\epsilon}{\hbar v} + \phi)} \quad (3.25)$$

In the case of a symmetric system, one can say that $t_1 = t_2$ and the Equation 3.25 becomes:

$$T(\epsilon, \Phi) = \frac{|t_1|^4}{1 + (1 - t_1)^4 - 2(1 - t_1)^2 \cos(2\pi \frac{\Phi}{\Phi_0} + \frac{2L\epsilon}{\hbar v} + \phi)} \quad (3.26)$$

If one assume that the transmission and reflection coefficients are set arbitrarily at a mid-range value;

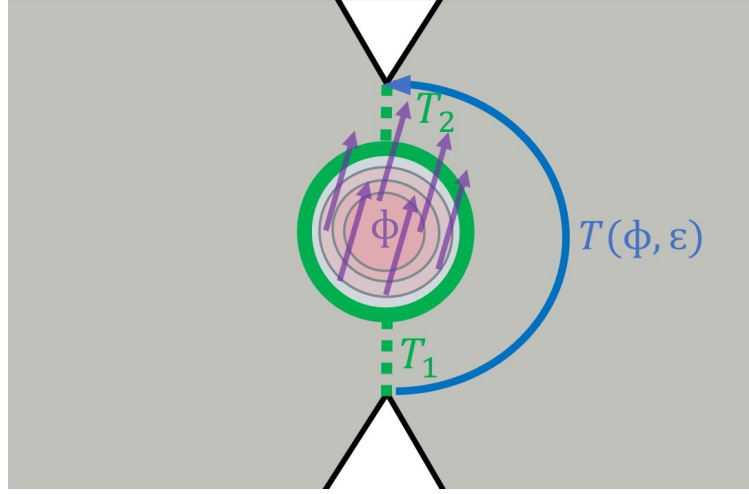


Figure 3.18: Schematic representation of transmission coefficient in the case of the single constriction. The blue arrow represents the total transmission from one edge to the other through the QHI. The green transmission dotted lines T_1 and T_2 are the intermediate transmission through QPCs.

$t_1 = r_1 = 0.5$, the Equation 3.27 is rewritten as:

$$T(\epsilon, \Phi) = \frac{0.0625}{1.0625 - 0.5 \cos(2\pi \frac{\Phi}{\Phi_0} + \frac{2L\epsilon}{\hbar v} + \phi)} \quad (3.27)$$

Assuming that $\frac{2L\epsilon}{\hbar v} + \phi$ is a phase constant one can obtain the transmission probability as a function of the magnetic quantum flux (Figure 3.19).

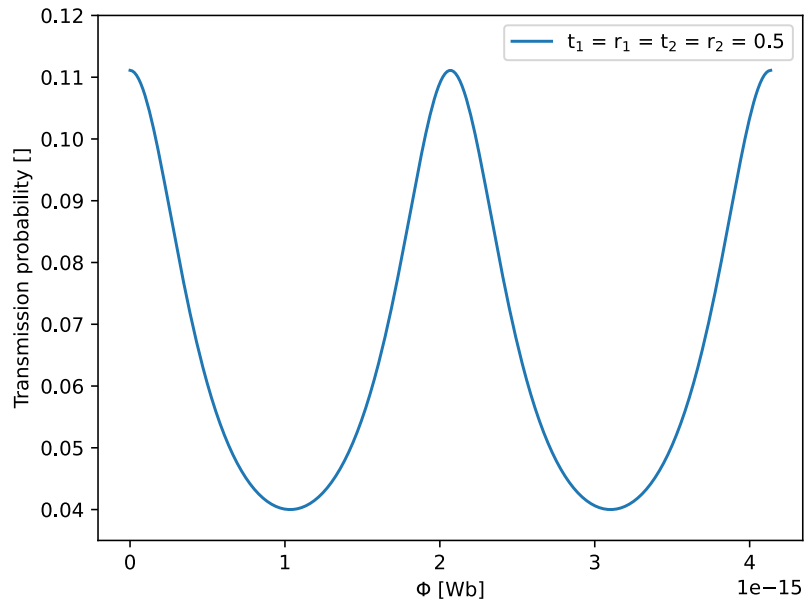


Figure 3.19: Transmission probability T as a function of the magnetic quantum flux Φ for the same reflection and transmission coefficient in both QPCs.

Several things are important to notice:

- The first one is to compare the oscillations on Figure 3.20 with the AB oscillations. Indeed, varying Φ is comparable to vary B because there are linked by the following formula:

$$\Phi = B \cdot A \quad (3.28)$$

In that case by changing Φ , B is also changing because A is maintain constant. As introduced in previous section, the AB effect is highlighted by changing B hence one can say that the oscillations represented on Figure 3.19 are comparable as AB oscillations.

- A second thing is to compare that results with Figure 3.17. The difference between both graphs is that on Figure 3.19, the coupling parameters are not changing unlike the other graph. The oscillations are only due to the variation of the magnetic quantum flux in the cavity. On the other hand, on the Figure 3.17, there is a change of coupling parameters due to the change of the tip potential size. It can be understood by looking at the Figure 3.20. Indeed, the transition from the green to the red line is made by increasing the transmission parameter as well as the tip potential width. One can see that the transmission probability is increasing which explains the variation of resistance on Figure 3.17 in addition to the change of quantum magnetic flux inside the cavity.

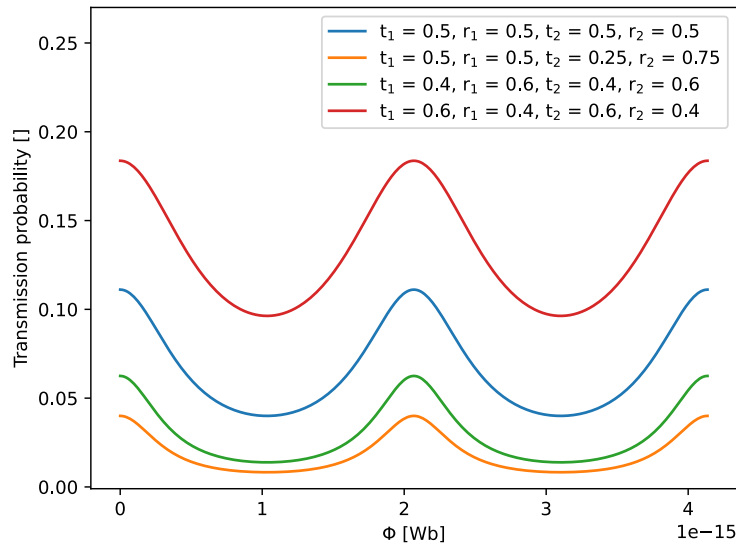


Figure 3.20: Comparison of transmission probability according to the magnetic quantum flux for different value of reflection and transmission coefficients. The red, blue and green curves correspond to a tip placed at the center with different width traduced by a change of transmission and reflection coefficient. The orange curve corresponds to an asymmetric system with tip not placed at the center. In that case the coefficients are not the same for the two QPCs.

3.5 Double constriction

The double constriction Hall bar design is represented on Figure 3.22. As for the first Hall bar, the amplitude of the tip potential is set at 0.05 eV, and both length and width are respectively 1 μ and 500 nm. The distance between the two constrictions is 500 nm. In this experiment, a critical parameter is what has been called the constriction aperture: it is the vertical distance between two apex. On the Figure, it is labeled and measured at 30 nm.

As stated in the section 3.3, the paper of C. Deprez et al. has been a great inspiration for this design. They used plunger gates in a Fabry-Pérot cavity in order to move the trajectory of the interfering edge channel and to modulate the effective interferometer areas. However, the idea for this work was to bring a twist to their original experiment. As for the simple constriction, the SGM will be used to locally gate a region of choice of the cavity. As a matter of fact, replacing these plunger gates by the polarized SGM tip has some benefits. Firstly, from a fabrication point of view. The process is arduous enough, random for some parts and depends already on many factors that can alter the final result. SGM also offers more freedom on the positioning of the potential perturbation.

An appropriate constriction aperture make the experiment possible. In fact, the area between the two constrictions can be seen as Fabry-Pérot cavity. For interferences to be observed, the cavity edges have to act like semi-reflecting mirrors. There would be not point in having perfect transmission at the two interfaces.

The same comment has to be made here. The reflection/transmission are set by this constriction aperture. Indeed, the more narrow the aperture is, the more electronic backscattering there will be. To generate clear patterns of interferences, a medium value of reflection coefficient is the appropriate choice. Essentially, if this coefficient is set too high, there is not much current flowing through the first gate. If the coefficient is set too low, there is only a small portion of the total current trapped in the cavity available for interferences.

On Figure 3.21, a simulation run for R_{xx} as a function of the constriction aperture. This resistance is directly linked to the reflection coefficient of the constriction. The backscattering starts at about 230 nm indentation depth, which is 40 nm of aperture ($500 - 230 \cdot 2$ nm). After testing different values with current density diagrams, the choice of 30 nm has been made. This value generated enough reflection at both gates.

3.5.1 Comparison with the simple constriction design

There are several distinctions between the two Hall bar design that make each of them interesting in their own way. The main difference is that the potential imposes in some way the reflection/transmission through the constriction in the single constriction Hall bar. Without this QHI, the transmission is constant along the bar. Therefore, this tip plays a double role in the single constriction experiment: it tunes the proportion of charge carriers transmitted through the QPC and hence generates the AB oscillations. However, in the double constriction, these two points are separated. The reflection/transmission is only determined by the constriction aperture as well as the AB oscillations are only determined by the size of the potential.

Speaking of Aharonov-Bohm oscillations, this time the area intercepting the quantum flux does not correspond to the surface of the potential. In fact, it is the loop of current flowing on the edges of

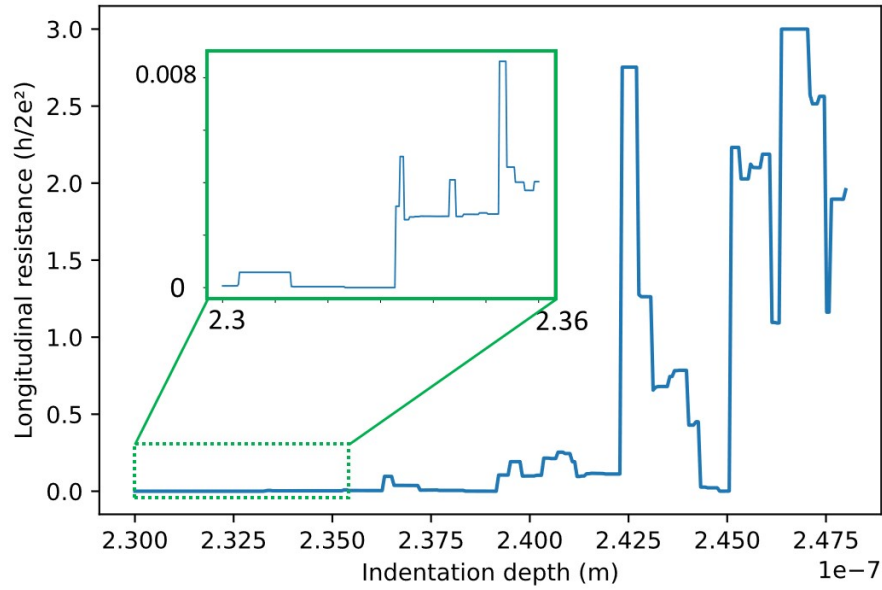


Figure 3.21: R_{xx} as a function of the indentation depth in a single constriction and with no tip potential applied. The green inset shows a zoom where the first charge carriers are reflected.

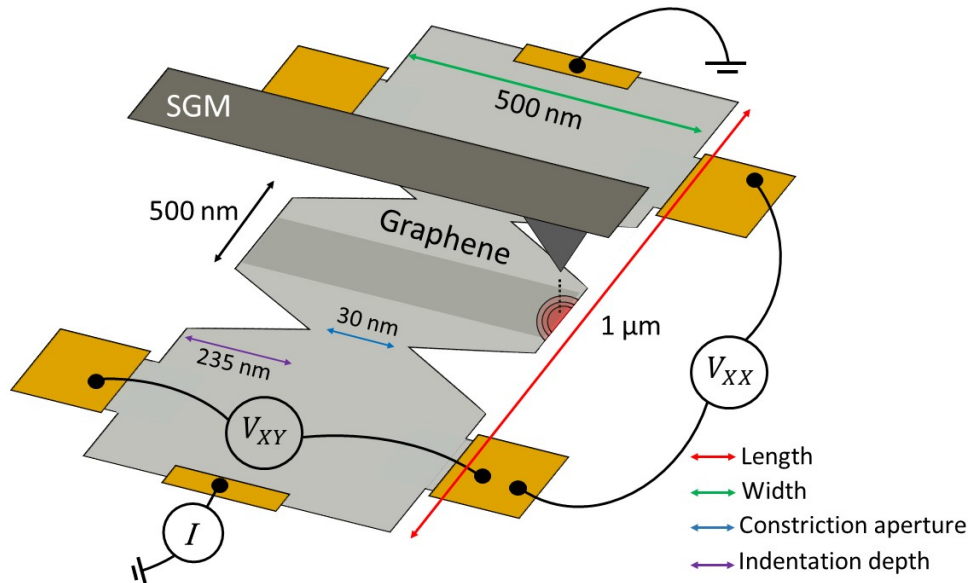


Figure 3.22: Schematic view of the double constriction with the SGM tip potential on the edge between the constrictions at $B = 8$ T.

the cavity (Figure 3.23). Nevertheless, varying the size of the potential also varies the area of this loop. Interferences are still created because of the applied potential.

3.5.2 Evolution of the longitudinal resistance with the tip potential width

As in the previous section 3.4.3, R_{xx} is computed as a function of the potential width. The tip is placed above the edge in order to form a semi-disk. That way, it is similar to a side gate. The Figure

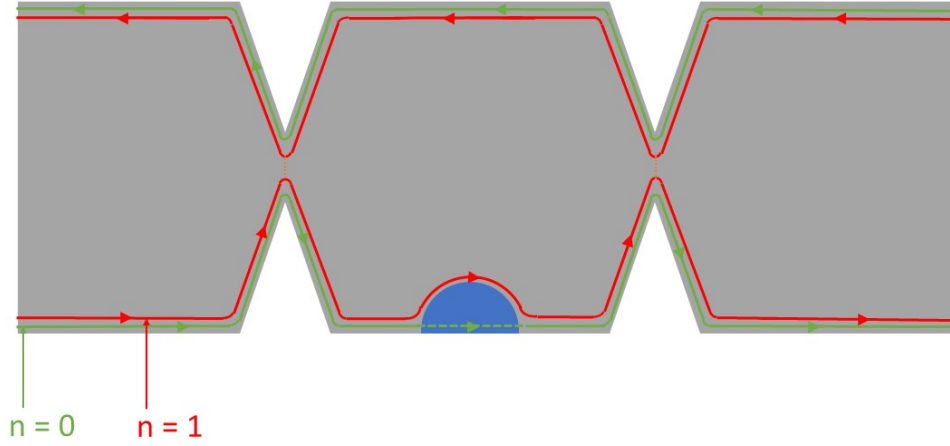


Figure 3.23: Schematic representation of the directions of the edge channels $n = 0, 1$ with the tip potential in blue for the double constriction.

[3.24](#) might help to get a clearer view of the simulation.

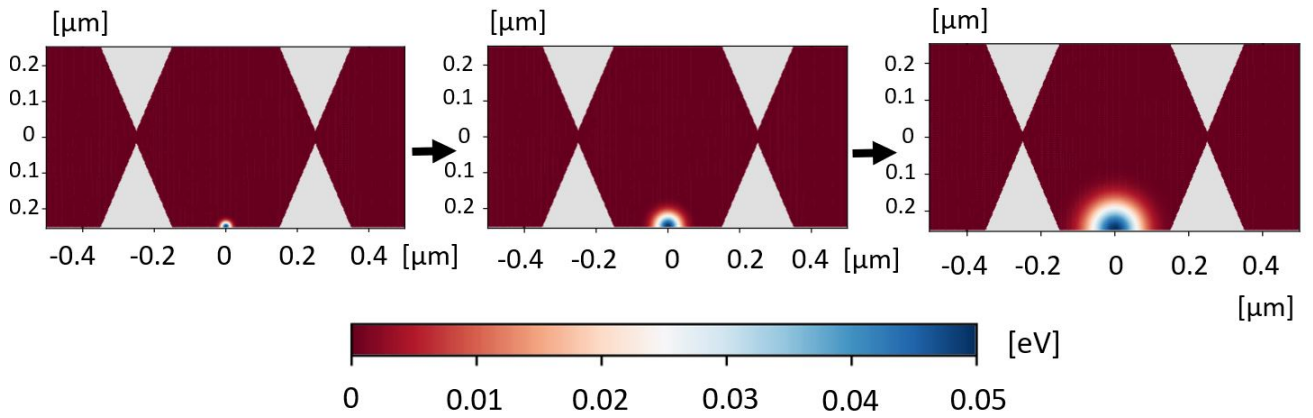


Figure 3.24: Heat map of the evolution of the width of the tip potential.

These simulations will be separated in two different experiments in the following sections. The first one is focused on finding the right parameters in order to involve only the edge channel $n = 0$ creating a NPN junction. The second part is focused on more exotic N/N'/N junctions dealing with several edge channels.

3.5.3 Configuration for one edge channel

The following set of parameters gives the energy levels configuration of [Figure 3.25](#).

- Tip potential $V_{tip} = 0.2$ eV
- Magnetic field $B = 10$ T

- Scaling $s = 8$
- Fermi energy $E_F = 0.15$ eV
- Constriction aperture = 30 nm. The Hall bar is symmetrical, so both constrictions have the same aperture.

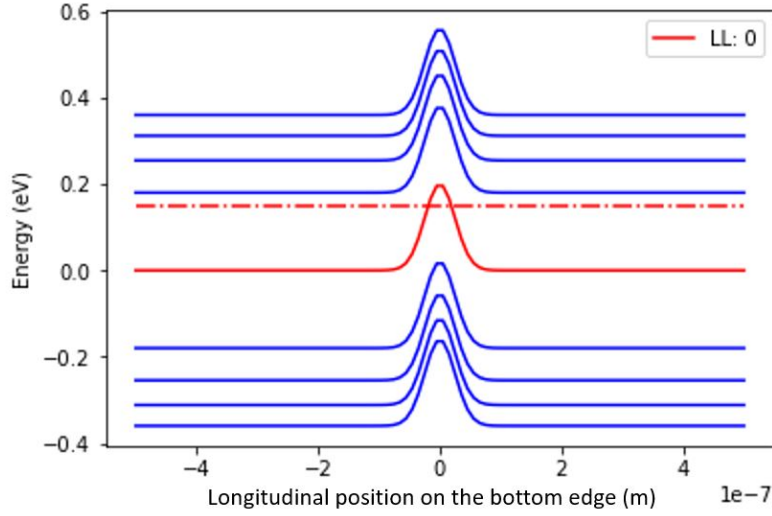


Figure 3.25: Energy of the Landau levels with the chosen parameters. It is a cross-section along the length of the Hall bar.

On Figure 3.26, the simulation run for R_{xx} as a function of the potential width. This curve has to be compared with the curve of Figure 3.10. In this case, there is no global increase of R_{xx} . It can be justify by the fact that the coupling between the potential tip and the edge channel is not evolving during this simulation. The bump of potential is shaping the energetic landscape in a way that the channel is forced to flow around it. In contrast with the single constriction where the carriers has to tunnel to join the circular edge channel. Furthermore, the amplitude of the oscillations is constant for this experiment. Once again, it is expected as there is no variation of coupling.

Concerning the oscillations a shift in the frequency is observed at around 37 nm and 58 nm. It seems to be an unexpected supplementary peak. At this time, no definite explanation has been given for this effect. An assumption is that this peak is linked to interaction between hole and electron current around the NPN junction.

3.5.4 Configuration for two edge channels

The goal of this simulation is to add another component to the previous regime of Figure 3.26. For this purpose, a 6/2/6 junction has been imagined. Indeed, edge channels $n = 0, 1$ are at stake in this configuration. However, parameters are specifically picked for the channel $n = 1$ to cross the Fermi energy but not the $n = 0$. In other words, in the cavity, there will be a channel deviated by the tip potential and the other following its original trajectory (this is the green channel in Figure 3.23). Here are the set of parameters chosen:

- Tip potential $V_{tip} = 0.05$ eV
- Magnetic field $B = 8$ T

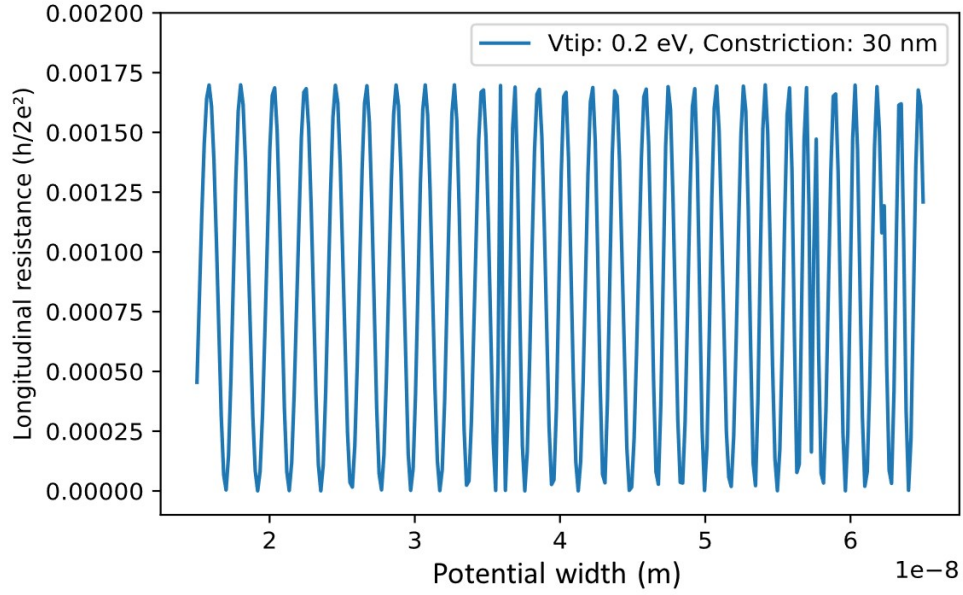


Figure 3.26: Longitudinal resistance as a function of the potential width for the double constriction.

- Scaling $s = 8$
- Fermi energy $E_F = 0.175$ eV. It corresponds to the highest value of Fermi energy possible in the linear regime of graphene (equation 3.20).
- Constriction size = 30 nm. Both constrictions have the same aperture.

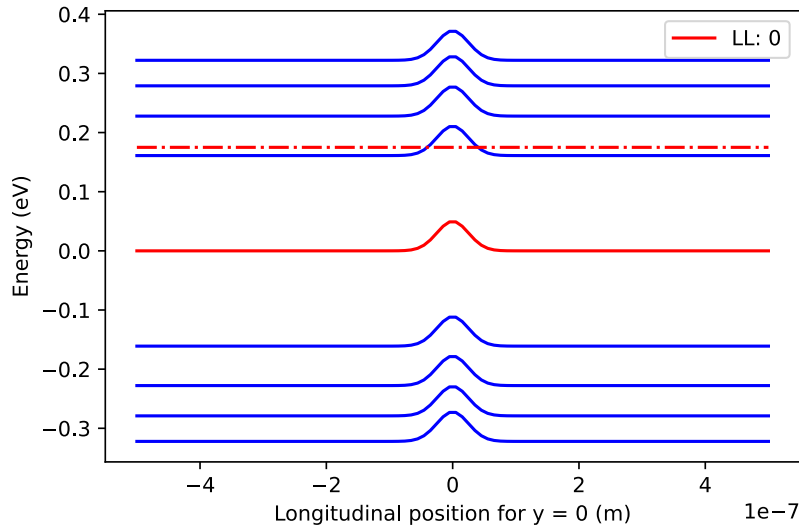


Figure 3.27: Energy of the LL with the chosen parameters. The Fermi energy crosses the edge channel $n = 1$ to form a $6/2/6$ junction. The graph corresponds to a cross-section along the length of the Hall bar.

The result for this simulation is presented on Figure 3.28.

Astonishingly, the curve is quite complex and many things have to be noticed. The global shape

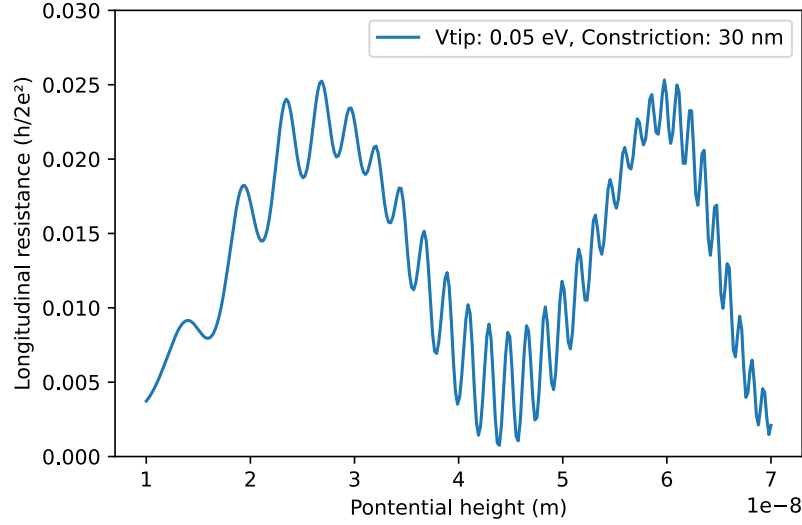


Figure 3.28: Longitudinal resistance versus the potential width for two edge channels.

seems to be a low frequency sinusoid. On this curve, another sinusoid is modulated. Its frequency is increasing with the potential width and its amplitude is also varying. There is no quick explanation for this graph. In the hopes of a better understanding of what is going on, the graph 3.28 is split into its two components. Indeed, the goal is to simulate and compute individually both resistive contribution of the channel $n = 0$ and $n = 1$.

- $n = 0$ channel component: At first glance of Figure 3.27, one could think that $n = 0$ lead to a constant R_{xx} component for any potential width. Because there is no crossing with the Fermi energy, the LL should not be deviated by the potential. Actually, there is a parameter to take into account: the density of states near the potential. This parameter affects the wavelength of the edge channel.

To simulate only this component, LL $n = 0$ and 1 are set on both sides of the Fermi level. Therefore, exclusively the $n = 0$ edge state is excited. The potential tip is set at 0.15 eV but is not high enough to cross $n = 1$. The other parameters are the same as section 3.5.4. Energy bands are represented on Figure 3.29. The simulation result is shown on Figure 3.30. This time, sinusoidal oscillations are not signature of AB effect. In fact, the variation of the wavelength of $n = 1$ with the potential width generate interferences in the cavity. The amplitude is kept constant as the backscattering with the counter-propagating edge is not modified. However, the frequency is increasing with the potential width. This curve can be modeled by:

$$R_{xx, n=0}(w) = A_{n=0} \cdot \sin(2\pi \cdot f_{n=0} \cdot w^2) \quad (3.29)$$

where $A_{n=0}$ is the amplitude, $f_{n=0}$ the initial frequency and w the potential width. One notice that increasing the magnitude of V_{tip} also increases the frequency of the R_{xx} curve.

- $n = 1$ channel component: For this configuration, the geometry of the sample has to be switched (Figure 3.31). Indeed, the goal is to find a way to interfere the LL $n = 1$ in the cavity while keeping $n = 0$ fully transmitted. A simple way to do that is to etched replace the constrictions by triangle shaped fixed potentials. For $n = 1$, the experiment is exactly the same as the one of Figure 3.27. However, the $n = 0$ channel is transmitted through the triangle shaped regions.

On Figure 3.32, the energy diagram along the x -axis. The potential in the triangles is steep

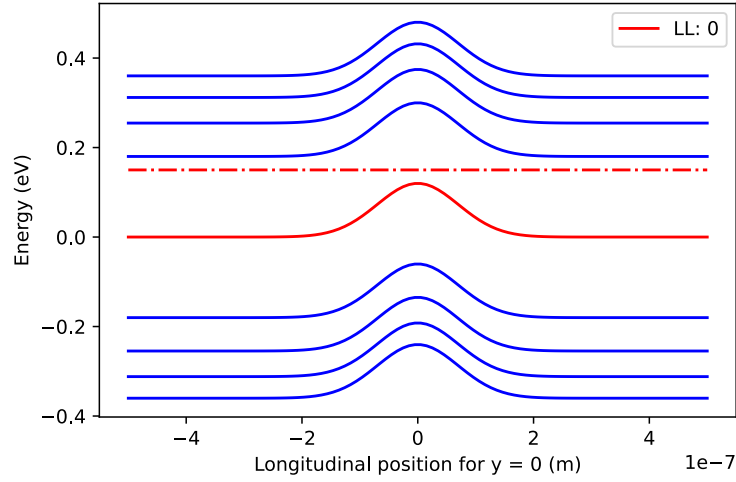


Figure 3.29: Energy bands configuration where only LL $n = 0$ is excited.

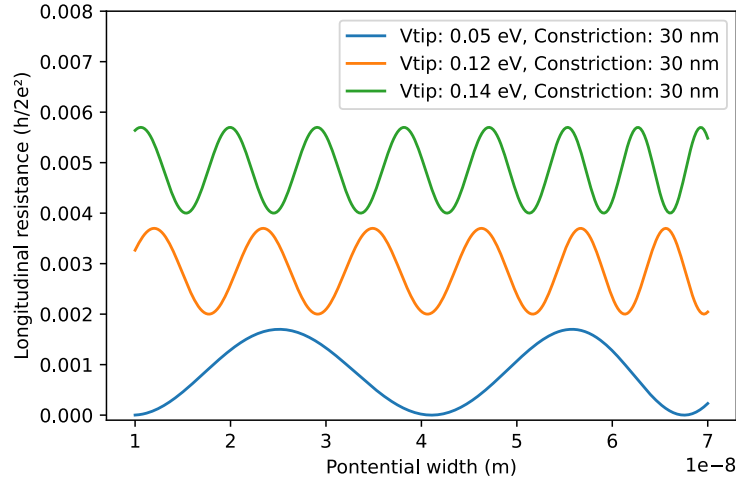


Figure 3.30: R_{xx} as a function of the potential width for several $V_{tip} = 0.05, 0.12, 0.14$ eV with a constriction aperture of 30 nm. The orange and green curves are offset by respectively 0.002 and 0.004 $\frac{h}{2e^2}$.

and constant on its section. The parameters chosen to obtain that kind of configuration are the following:

- Tip potential $V_{tip} = 0.05$ eV
- Triangles potentials $V_{triangle} = 0.05$ eV
- Magnetic field $B = 8$ T
- Scaling $s = 8$
- Fermi energy $E_F = 0.175$ eV. It corresponds to the highest value of Fermi energy possible in the linear regime of graphene (equation 3.20).
- Constriction size obtained with the triangles potentials = 30 nm. Both constrictions have the same aperture.

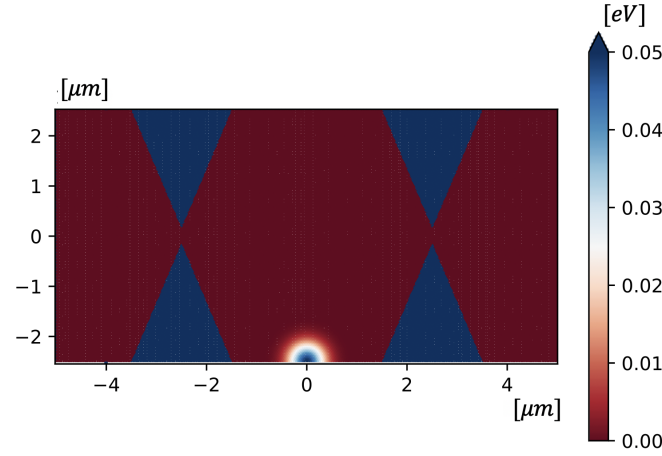


Figure 3.31: Schematic representation of the geometry to compute the $n = 1$ channel component of the graph [3.28](#). Compared to the previous geometry, the constrictions are replaced by triangle shaped potentials.

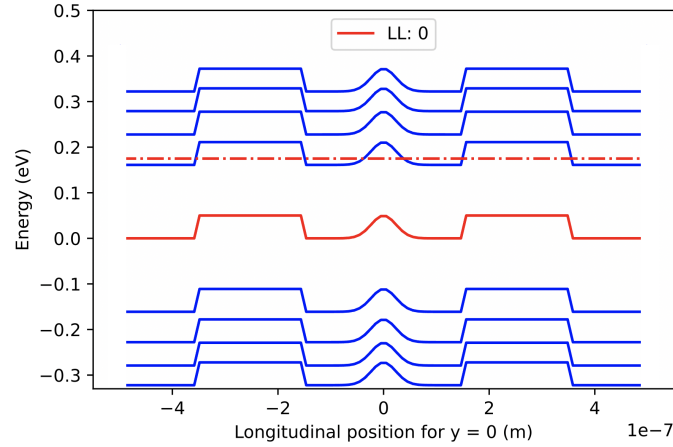


Figure 3.32: Energy diagram at the bottom of the sample. Only the channel $n=1$ will be affected by triangles potentials and by the Gaussian tip potential at the center of the device.

To verify the hypothesis on the trajectory of the channels, the current density is computed on Figure [3.33](#). Unsurprisingly, a part of the total current is following the potential landscape : that is $n = 1$. A part is flowing along the edge through the basis of the triangles: that is $n = 0$. Thus, $n = 0$ is too far to interact with its counter-propagating channel while $n = 0$ is able to loop in the cavity and interact with its counter-propagating channel.

By repeating the same simulation as for the Figure [3.28](#), the new R_{xx} curve is obtained in Figure [3.34](#). The signature of AB oscillations is retrieved once again because of the variation of the path length of electrons. Nevertheless, the amplitude of R_{xx} is very small (about 5 orders of magnitude below) in comparison with previous simulations. In fact, it seems like the potential constrictions do not reflect much current although the aperture is kept at 30 nm. Figure [3.33](#) attests the lack of backscattering at each gate. At this point, there is no

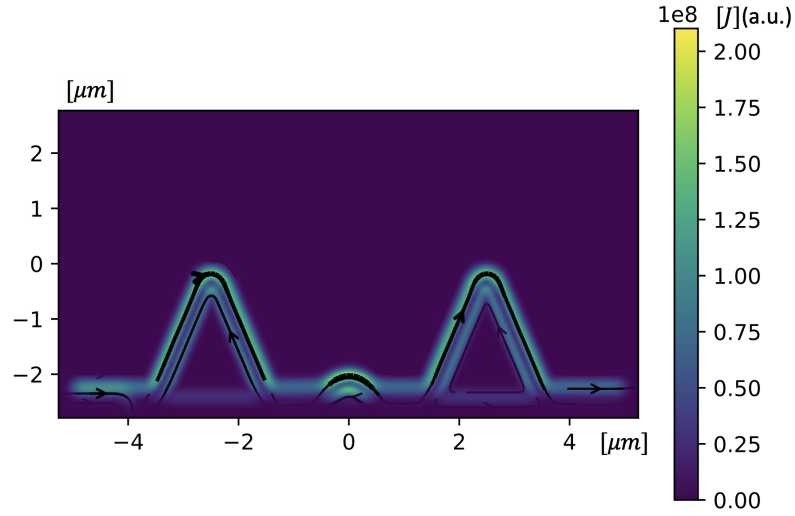


Figure 3.33: Heat map of the current density in this new geometry. One can see current deviated by the triangles potentials corresponding to channel $n = 1$ and current not deviated belonging to channel $n = 0$.

straightforward explanation for this.

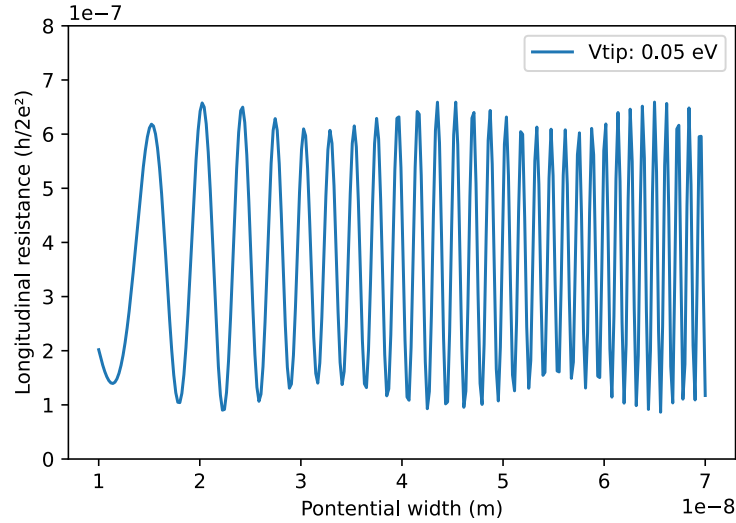


Figure 3.34: R_{xx} as function of the potential width for the channel $n = 1$.

To retrieve the graph of Figure 3.28, one need to sum the two different components of the total resistance. Unfortunately, the $n = 1$ component is minor in comparison to $n = 0$. The total curve is pretty much the one Figure 3.30 for $V_{tip} = 0.05$ eV. Nevertheless, one can imagine that small R_{xx} curve would have larger amplitude oscillations with a higher reflection coefficient at its constrictions. This is why it should be interesting to multiply these values to enter the same range of R_{xx} as Figure 3.31. Figure 3.35 shows the total R_{xx} with the small oscillations multiplied by 10^3 . This curve is very close in several ways to the one of Figure 3.28. Both graphs show a sinusoid of high frequency modulated on another bigger sinusoid of lower frequency. In addition, the frequency of the two sine waves is raising with the potential width. The similarities allow to validate the model for the

decomposition in $n = 0$ and $n = 1$ described in this section.

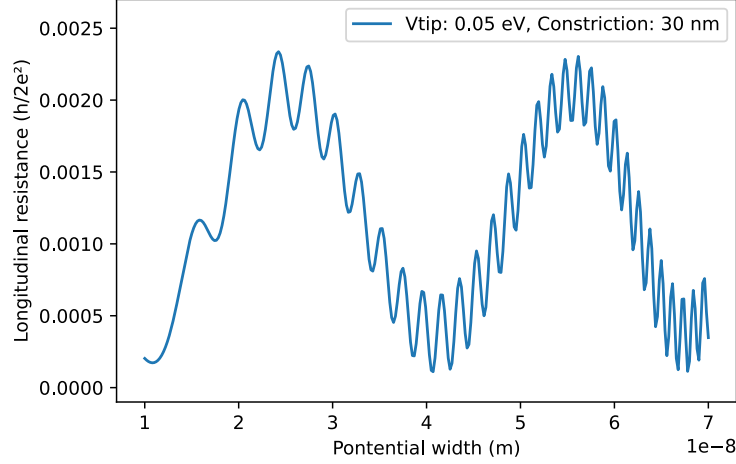


Figure 3.35: R_{xx} as a function of the potential width computed by adding both contributions (channel $n = 0$ and $n = 1$). The resistance values of Figure 3.34 are multiplied by a factor 1000 in order to observe its component.

In a more mathematical perspective, the general curve of Figure 3.28 (noted $R_{xx,6/2/6}(w)$) can be modeled by:

$$R_{xx,6/2/6}(w) = R_{xx,n=0}(w) + R_{xx,n=1}(w) = A_{n=0} \cdot \sin(2\pi \cdot f_{n=0} \cdot w^2) + A_{n=1} \cdot \sin(2\pi \cdot f_{n=1} \cdot w^2) \quad (3.30)$$

3.5.5 Configuration for more than two edge channels

Simulations for more than two edge channels is possible. The Figure 3.36 is an example of such a situation with three edge channels at stake. With the following parameters, the bump of potential forms a 10/6/10 junction.

- Tip potential $V_{tip} = 0.05$ eV
- Magnetic field $B = 4$ T
- Scaling $s = 8$
- Fermi energy $E_F = 0.175$ eV. It corresponds to the highest value of Fermi energy possible in the linear regime of graphene (equation 3.20).
- Constriction size = 30 nm. Both constrictions have same aperture.

In that case three contributions of interference must be taken into account. Each edge channel has its own contribution to interference. The smallest oscillations are due to channels $n = 2$. Indeed, since the Fermi energy is crossing the energy state number two at the tip, it is the only one that can interact with the potential. In that case, the AB oscillations appears for that level because there is a change of the intercept magnetic field area. For channels $n = 0$ and $n = 1$, the potential will change the DOS like in Figure 3.31. The sum of that three components will lead to a graph like the Figure 3.37. Obviously, the curve is more complex to evaluate but it is the kind of result expected from experimental data.

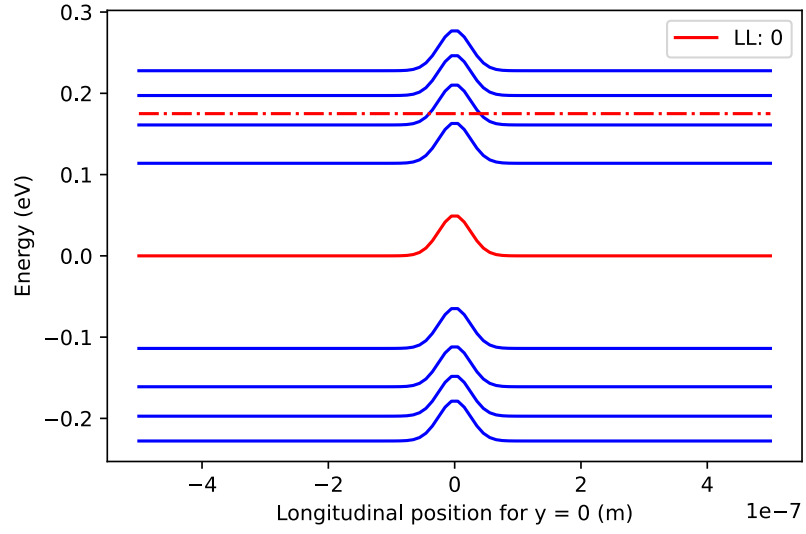


Figure 3.36: Energies of LL for a configuration with edge channels $n = 0, 1$ and 2 excited.

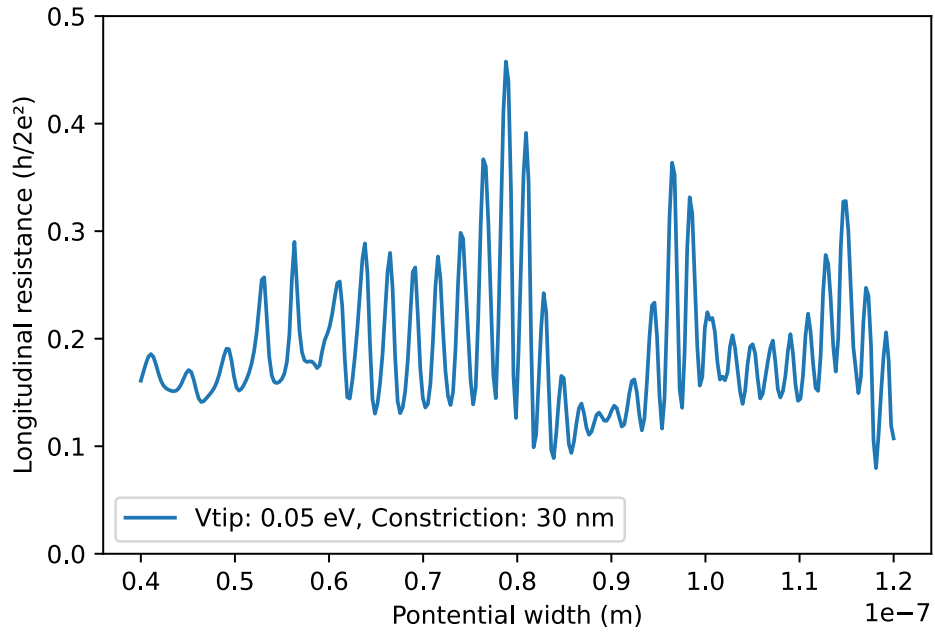


Figure 3.37: R_{xx} as a function of the potential width for the 10/6/10 junction.

Chapter 4

Fabrication process

This chapter is dedicated to detail every steps of the fabrication process of the devices. Indeed, the decision of building two different graphene heterostructures (stacks) has been taken in order to highlight interferences of different origins. The structural characterization as well as the final product will be described.

Fabrication steps until the e-beam lithography have all been realized in *Winfab* cleanroom of UCLouvain. The remaining steps to the final stack have been realized in the laboratory of Université de Paris.

4.1 Device architecture

The starting point of both devices is a Hall bar, already largely studied in the literature. As the interferences at stake are between a propagating edge channel and its counterpropagating channel, constriction will be etched in the stack. It will allow to narrow the distance between these two channels and make them interact (with or without the tip of the SGM depending on the experiment).

4.1.1 First stack

The first stack consists of a Hall bar with 8 lateral contacts and 2 longitudinal contacts with a constriction at the half-length. The lateral contacts number have been doubled compared to a classical Hall bar because the size of the exfoliated materials allowed it. The second one on each side serve as a back-up if the first one does not work. The dimensions (see Figure 4.1) have been chosen to respect the graphene and BN size, to avoid being under wrinkles of the BN and to separate the contacts with at least $1\text{ }\mu\text{m}$ (to avoid short-circuit between them). The constriction aperture is theoretically set to 350nm . In this experiment, the tip potential of the SGM can be tuned to couple the propagating and counterpropagating channels at the center of the constriction. Therefore, the aperture can be overestimated just to make sure the lithography process will not merge both apex of the constriction.

The vdW heterostructure compound layers (graphene and BN) have been synthesized by mechanical exfoliation starting from macroscopic flakes. The stack is then transferred on gold-marked wafer used

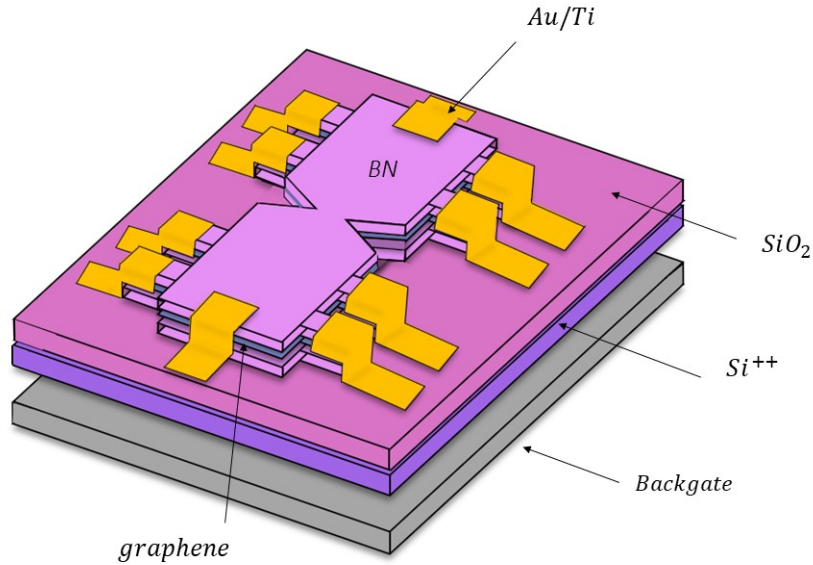


Figure 4.1: Schematic design of the first stack on its substrate. The encapsulated graphene is shaped in a Hall bar with metallized contacts.

to locate the structure in the lithography process. The wafer is composed of 90 nm-thick SiO_2 layer on a P-doped Si layer deposited on a Al layer used as a back-gate.

4.1.2 Second stack

The second stack is also based on a Hall bar with back-up lateral contacts. The main difference with the first stack is that there are two constrictions in series. In the experiments with this stack, the SGM tip is placed on a edge between the two constrictions. In this case, the constriction aperture must be shorter. Indeed, each constriction can be seen as QPC with parameters computing the probability of transmission and reflection. These apertures are set to 250 nm which is in theory too large for any backscattering. To overcome this issue, triangular side gates on each side of the constrictions are etched. Ideally, applying tension in these gates would deflect the edges channels from their original path and therefore bring them closer. Otherwise, the dimensions of the stack follow the same rules as the first one and the substrate with the back-gate remains the same. The design is described on Figure 4.2.

4.2 Graphene and thin BN production techniques

4.2.1 Graphene production

This section is based on [8]. Since first graphene production by the Novoselov research group in 2004 by mechanical exfoliation, many techniques have been developed. These techniques distinguish themselves by the quality, the ease and the cost to produce a monolayer. The most used ones are shortly described in the following [52]:

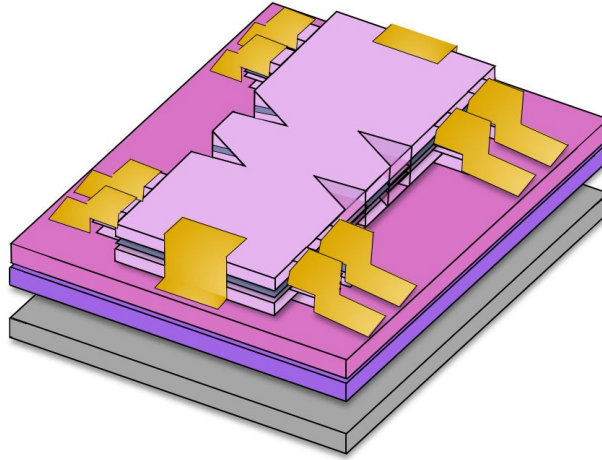


Figure 4.2: Schematic design of the double constriction sample.

- **Graphite sonication:** The principle is based on graphite exfoliation. Starting from graphite sheets disposed in organic solvents such as N-methyl-pyrrolidone. The solution is sonicated leading to exfoliated sheets of graphene. This is possible with solvents whose surface energy matches the one of graphene. Indeed, the surface tension of these solvents need to favor the total area of the graphite. The suspended sheets can be extracted using centrifugation. This technique can produce macro-scale graphene films in a short period of time. However, the charge carrier mobility is much lower than other techniques [53].
- **Epitaxy by CVD:** Graphene is grown on copper foils at temperatures around 1000°C by chemical vapor deposition of carbon using a mixture of methane and hydrogen which is called the precursor. At this temperature, the precursor decomposes and large domains of graphene form on the copper. Then, the graphene has to be transferred to the substrate of interest. This step can be challenging but this method demonstrates high flake quality and size [54] [epi2].
- **Epitaxy by heating SiC:** This technique is based on the sublimation of Si atoms in a silicon carbide wafer. In order to achieve that, this wafer is heated above 1000°C. The carbon atoms left behind form graphitized surfaces. Once again, an issue with this technique is the energy consumption needed to reach high temperatures. On the other hand, the size of the crystallites obtained can reach hundred micrometers, a proof of quality.
- **Mechanical exfoliation with tape:** This method is the one used in our work. It will be developed in the following section.

4.2.2 Mechanical exfoliation

As mentioned earlier the goal of this work is to demonstrate different electronic interferometry patterns. Amongst other parameters such as the size of the flake, those that interest us in this work are mainly the charge carrier mobility and the quality of the layer. Indeed, these parameters are focus in the electronic research field. Therefore, it has been shown that mechanical exfoliation is well-suited for this task.

The starting point is macroscopic natural flakes of graphite. Ideally, the idea behind this process is

to peel off graphene, layer by layer, from the bulk graphite. To overcome the vdW attraction between adjacent planes, mechanical normal or lateral force could theoretically be applied. Normal force creates a micromechanical cleavage [55] between two layers and shear force takes advantage of the self-lubricating properties of graphite to allow sliding between planes [56].

The path followed in this work is based on [52] which has been awarded by Nobel Prize in physics in 2010. To generate the cleavage, scotch tape is used between the top and bottom of the graphite. In reality, it is not possible to remove a single layer every time the tape is unglued. Indeed, the process has to be repeated. The flakes obtained at each step become thinner. In the end, those flakes have different thickness and some might be monolayers. Another important aspect is the fragmentation of the flakes following the exfoliation. Sure, it implies a smaller size of flakes but it increases the number of them. More flakes increases the chance to find graphene.

The exact process followed in this work is shown in detail in Figures [4.3], [4.4], [4.5], [4.6].

To start the exfoliation process, natural graphite flakes are laid down in line on a ~ 20 cm long Scotch Magic tapeTM strip. One side of the tape is stuck to the work station and the other is left free (see Figure [4.3a]). When several flakes form a line of about 2 cm or more, the tape is folded on itself at its half (see Figure [4.3b]). Pressure is applied on each side of the flake line with a laboratory nip (see Figure [4.3c]). Then, the tape has to be quickly peeled off from itself (see Figure [4.4d]).

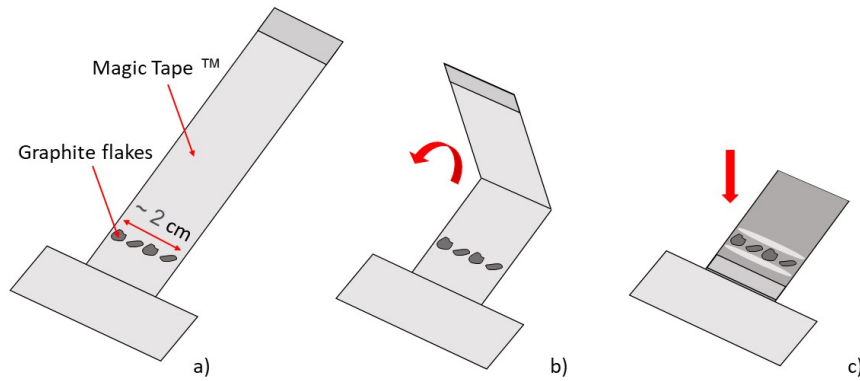


Figure 4.3

Graphite layers should appear on both sides of the tape, reducing the thickness of the starting flake. This operation has to be repeated about three times by shifting a bit the tape for the flakes not to overlap (see Figure [4.4e]). The tape should now have two surfaces of less shiny flakes of about 3 by 2 cm (see Figure [4.4f]).

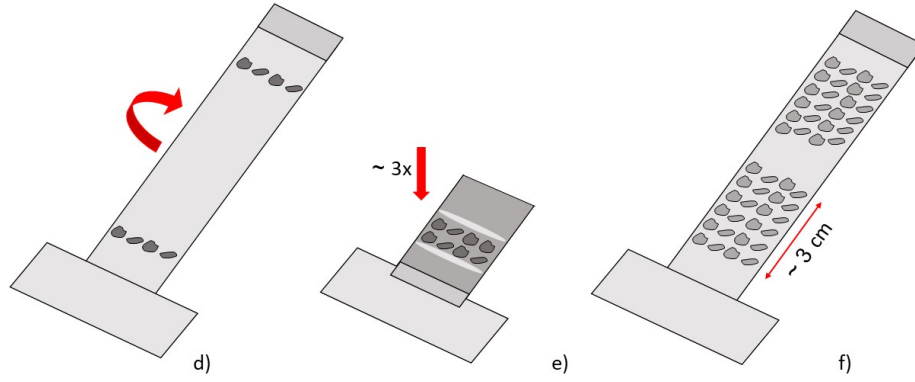


Figure 4.4

Two smaller tapes are laid down on the original long tape (see Figure 4.5g)). As this process relies on luck to a certain extent, these smaller tapes lead to a supplementary exfoliation and increase the number of flakes to analyze. If the original tape is cut in two halves, there are four small tapes that are placed sticky face up, on top of a glass slide. It is now time to drop Si/SiO_2 wafers, cleaned in acetone solution, on top of the flakes (see Figure 4.5h)). The flakes are in contact with the SiO_2 layer. Then, the glass slide is put on a heating plate at 90° for 10 minutes in order to homogenize the contact surface (see Figure 4.5i)).

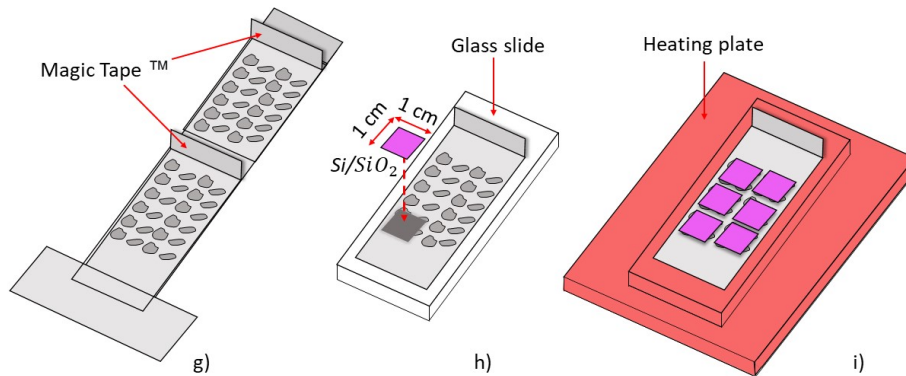


Figure 4.5

The last step consist of slowly removing the silicon wafers of the tape. For this purpose, the tape is flipped, sticky face down. With the help of a laboratory nip, a pressure is exerting on empty areas of the wafer. At the same time, gently pulling up the tape with fingers of the wafers one by one (see Figure 4.6j)). On the SiO_2 should remain a good amount of more or less thick graphite flakes.

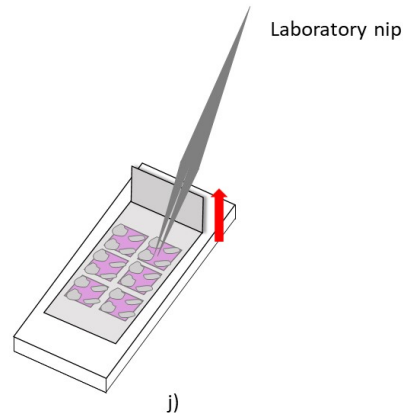


Figure 4.6

The silicon wafers are now ready to be examined under an optical microscope and the hunt for graphene begins.

4.2.3 Mechanical exfoliation of hBN

The process of exfoliation of the boron nitride relies on the same physical mechanism: creating cleavage between atomic planes bonded by vdW forces. However there are some variation in the technique linked to the scarcity and usage of BN.

The BN used are laboratory prepared flakes of few millimeters in size. A line of flakes is spread on a the same exact Magic tapeTM setup as for graphene exfoliation. But this time, the flake line should be about the size of Si/SiO_2 wafer, that is 1 cm (see Figure 4.7a)). Then, the scotch is fold on itself (see Figure 4.7b)). Pressure is applied on both side of the line with a laboratory nip (see Figure 4.7c)).

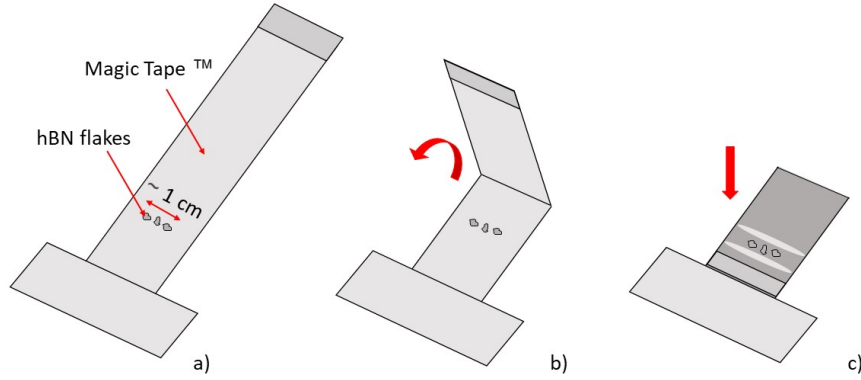


Figure 4.7

The tape is unfold (see Figure 4.8d)) and this folding operation is repeated about two times (see Figure 4.8e)) in order to have flakes aligned on 1 cm length on both sides (see Figure 4.8f)).

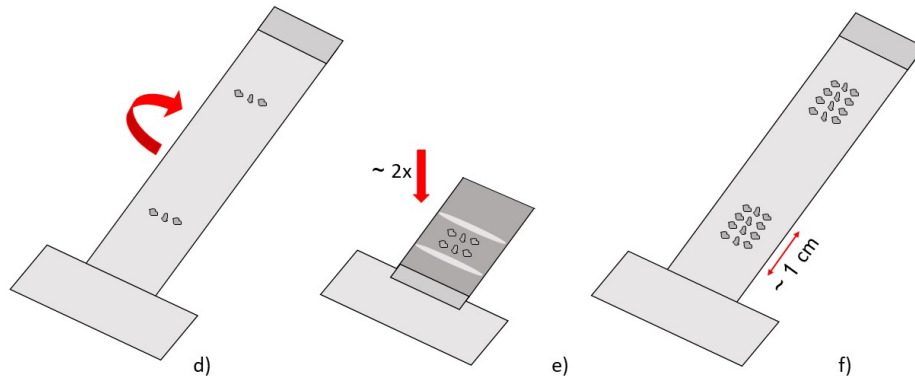


Figure 4.8

This time, Magic Greener tape TM is used to peel off the flakes (see Figure 4.9g)). The flakes that stuck on the original tape can be reused in the future for another batch of exfoliated BN. For this reason, these BN are covered by a piece of Greener tape.

The next step is also a bit different than the graphene process. Glass slide, cleaning and heating of the wafer is not needed here. In contrast with graphene, boron nitride flakes can be several layers thick. In fact, very thin BN is to be avoid; there are complicated to pick up in the following stacking process. Let us recall that BN purpose is to electrically insulate and protect graphene. However, too thick BN can be also constraining in the lithography process.

Therefore, 1 cm^2 Si/SiO_2 is stuck on the flakes (see Figure 4.9h)). Then, same as before, the tape is flipped and gently peeled off with the help of the nip (see Figure 4.9i)).

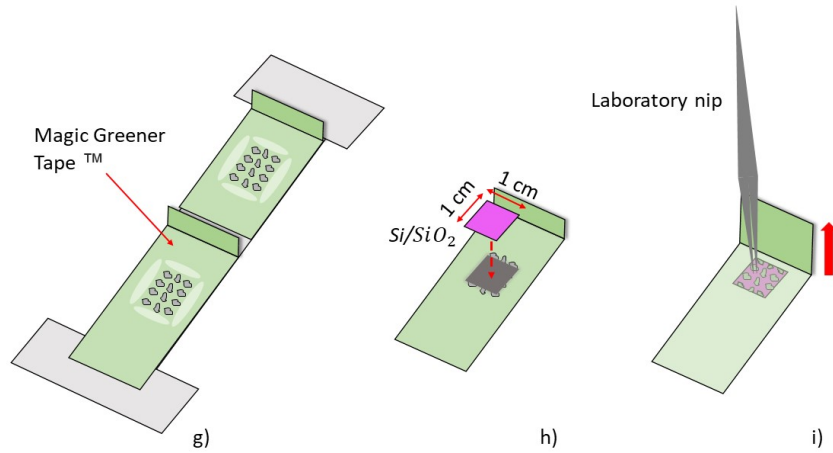


Figure 4.9

4.3 Graphene under optical microscope

There are several parameters to look for when searching for the perfect flake to use. First and foremost, the carbon-based flake needs to be very slightly colored. The thickness of graphite is directly linked to its transparency. Indeed, due to its unexpectedly high optical absorption of $\pi\alpha \approx 2,3\%$, monolayers of graphite contrast from the background. Identifying it is quite subtle but achievable. The Si/SiO_2 wafer is optimal for the observation thanks to its very high reflectivity. Thus, light passes through graphite twice and improve the contrast with the background. Color shifts are observed for thicker graphite due to interferences between the wafer and graphene layers.

In addition to its contrast, the flake requires an obvious homogeneity. As a matter of fact, electronic properties noticeably varies between single and double graphite layers [57].

Another requirement is the position of the flake. Indeed, the edges of the wafer are not suited for the transfer later on. In that case, once chooses the central part of the wafer, hundreds of micrometers away of the sides.

Last parameters of interest are the size and shape. As a conventional Hall bar is the intended design, the shape cannot be too short or too narrow. Naturally, in term of dimensions, the wider surface is to be looked for. There is the possibility to etch two different devices on the same flake if it is large enough.

On Figure 4.10 is shown a micrograph of the most convincing graphene flake from all the batches. Different things are noticeable. Starting from a global view, different size and thickness graphites are present on this x20 optical microscope lens zoom. A good thing is that the flake of interest, which is enclosed with blue dotted lines, is not located too close from the edges. For their part, the blue spots are tape glue residuals. The presumed graphene flake is shaped in a trapeze way with a width in the range of $20\text{ }\mu\text{m}$ and length above $100\text{ }\mu\text{m}$. Due to its compelling dimensions, one can imagine

etching two separated Hall bars on the length of this flake.

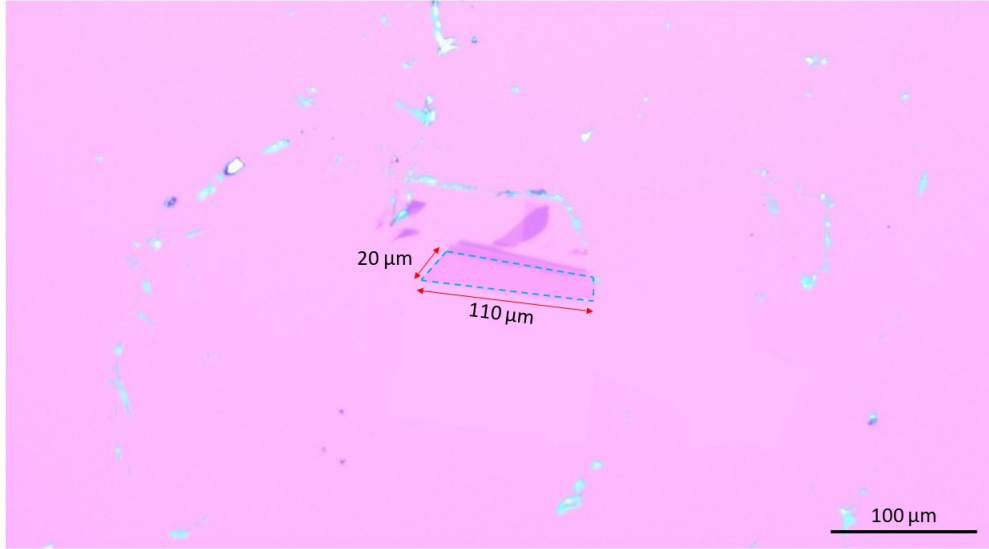


Figure 4.10: Optical microscope capture of a measured graphene flake.

Although the contrast of color between the background and the flake is slight, Raman spectroscopy will determine if it is really a single layer.

4.4 Raman spectroscopy

Raman spectroscopy is based on inelastic scattering between photons and matter. Due to its high sensitivity to physical and chemical properties of materials, Raman spectroscopy became an inescapable characterization tool in nanotechnology field [58]. In particular, this technique is very reliable and fast to determine the number of layers of graphitic materials. As other optical techniques, using photons also ensure a non-destructive and non-invasive analysis of materials.

4.4.1 Working principle

To collect information in a spectroscopic experiment, one needs to monitor the energy of photons reflected that has interacted with the material. Indeed, when a crystal is exposed to a light source, part of the photons are transmitted through it depending on the transmission coefficient and part of the photons interact with the lattice. These interactions are absorption or scattering processes depending on the vibration modes (i.e. phonons) and on the photon range of energies.

Considering the reflective processes, Rayleigh scattering is the predominantly elastic scattering. It corresponds to the multi-direction scattering of electromagnetic radiation from bound electrons, after being excited to virtual states far from resonance frequencies [59]. As it is an elastic process, the re-emitted photons are of same frequency as the incident photons.

However, some photons can interact with phonons or other excitations in the system. It causes a

shift up or down of the re-emitted photon frequency from the virtual state. These rarer events are called Raman scattering [60].

In Raman scattering, an increase of the wavelength from the reflected photon compared to the incident is called a Stokes shift. If the wavelength becomes smaller, it is called an anti-Stokes shift [58]. These energy shifts cause the electron to change its final energetic state from its original one. To conserve total energy, in the Stokes shift, the photons frequencies (and therefore their energy) lowering is accompanied with an electronic final state of the electron higher than the Rayleigh process. In the anti-Stokes shift, electrons finish in a lower state. A global view of the three mechanisms is represented in Figure 4.11.

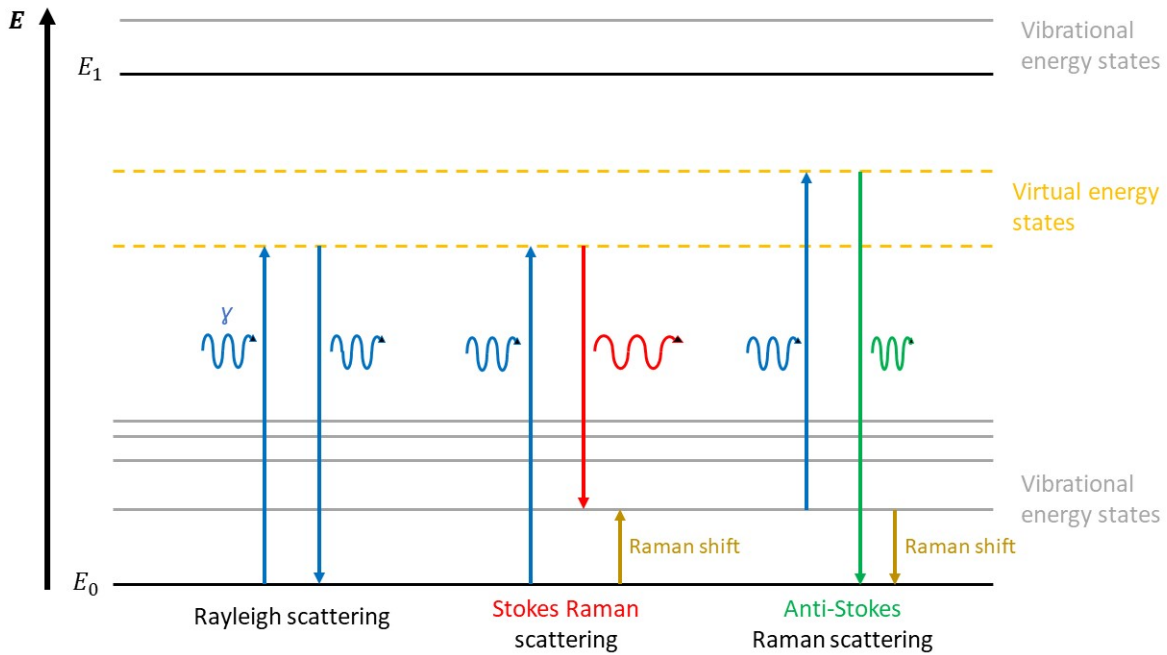


Figure 4.11: Representative electronic energy diagram of possibilities of light scattering. From left to right: Rayleigh scattering where the scattered photon keeps the same frequency as the incident one. Inelastic Stokes Raman scattering where the scattered photon has a lower frequency than the incident one. Inelastic anti-Stokes Raman scattering where the scattered photon has a greater frequency than the incident one.

Raman scattering depends on wavelength of incident radiation but the magnitude of Raman shifts does not depend on incident wavelength. Therefore, a Raman spectroscopy is an analysis of the intensity of the energy shifts as function of the incident photon wavelength. These Raman spectra graphs are expressed in terms of wavenumber notation, which is common for phonons, in units of cm^{-1} [61]. Since wavelength is often expressed in units of nanometers, Raman shift formula can be scaled explicitly like [62] :

$$\Delta\tilde{\nu} [cm^{-1}] = \left[\frac{1}{\lambda_i[nm]} - \frac{1}{\lambda_s[nm]} \right] * \frac{[10^7 nm]}{[cm]} \quad (4.1)$$

where λ_i is the wavelength of the excitation laser and λ_s is the wavelength of the collected scattered photons. With the help of Figure 4.11, one can identify that:

- If $\Delta\tilde{\nu} > 0$: Stokes Raman scattering
- If $\Delta\tilde{\nu} < 0$: Anti-Stokes Raman shift

In fact, positive Raman shifts are the most probable. These are the ones that are conventionally measured in Raman spectroscopy. To choose the right laser, one must take two parameters into account: sensitivity and spatial resolution. Indeed, Raman intensity is proportional to $\frac{1}{\lambda^4}$ and diffraction limit of the laser spot diameter is proportional to λ [63]. So, different lasers are adapted for different types of materials. For carbon-based materials, green and red lasers are best suited with 514nm and 633nm commonly used.

4.4.2 Raman setup

A typical Raman spectroscopy setup is represented on Figure 4.12. The experiment is run in a temperature controlled room with as little light as possible. Indeed, the laser has to be maintained stable and no other photon source has to interact in the process. In this experiment, the green commonly used 514nm laser is chosen. The first step is to find the flake on the wafer with the x100 objective of the microscope. Once it is calibrated, the laser is directed to the objective via mirrors and a beamsplitter. The re-emitted photons of different frequencies are collected in opposite direction. Behind the beamsplitter, they are focused with a lens to a filter. This filter is essential to get rid of the photons coming from Rayleigh scattering. A notch filter is the ideal candidate to transmit higher and lower frequencies while removing the primary frequency [64]. These filters allow data capture of the anti-Stokes and Stokes spectra down to $\sim 30 \text{ cm}^{-1}$. However, as they are expensive and their life span is short, wide pass-band filters are frequently used. Besides removing Rayleigh scattering, they also remove the anti-Stokes component. As said above, the Stokes component is sufficient to perform the analysis. After that, the Stokes Raman radiations scattered by the sample are separated from one another by a grating. Finally, the acquisition part is realized by silicon-based semiconductors CCDs [65]. They are photosensitive thus converting different photons in different electrical charges that are further read by an analog-to-digital converter.

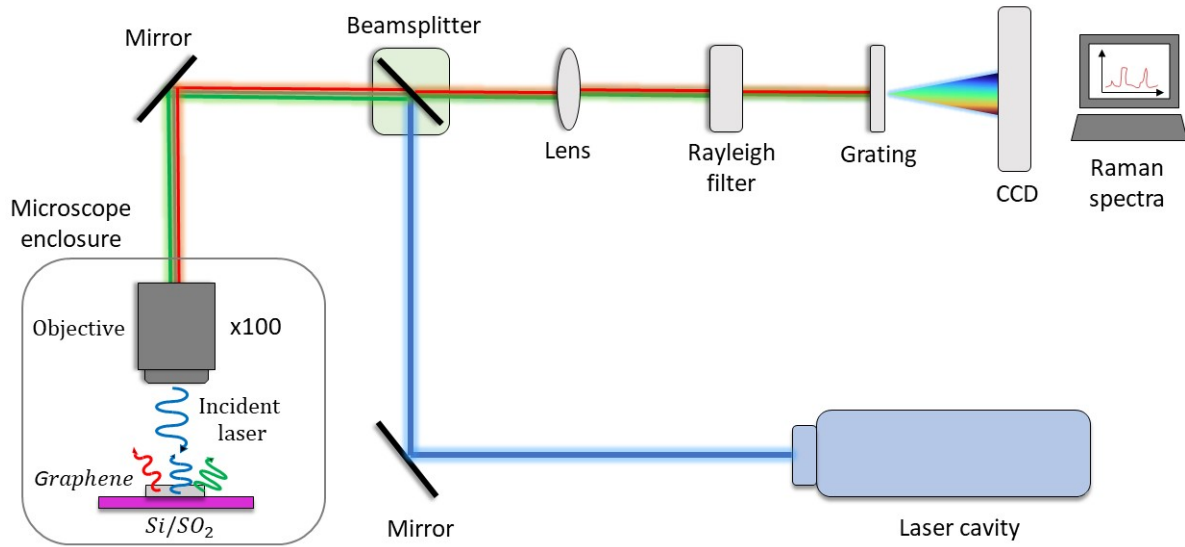


Figure 4.12: Representative scheme of a typical Raman spectroscopy setup. Adapted from [66]

4.4.3 Raman spectroscopy for graphene

Theory:

An interesting comparison is between pristine graphene and defected graphene in Figure 4.13. To understand the origin of the different peaks, it is insightful to have a look at the possible elementary steps of the Raman processes. Limiting the analysis to spectra up to $\sim 3000 \text{ cm}^{-1}$, peaks arise from one or two-phonons processes. Electron dispersion of occupied bands schemes in Figure 4.13 will help to understand the peaks. Four of them will be discussed in this section as they are the most relevant for graphitic materials.

- **D-peak** at $\sim 1350 \text{ cm}^{-1}$: This peak requires defects for its activation. Transverse optical phonons around the Brillouin zone corner **K** causes breathing modes of the 6-atoms carbon hexagon. It is the signature of a poor quality of the graphene.
- **G-peak** at $\sim 1580 \text{ cm}^{-1}$: This peak can be found in all graphitic Raman spectrum. It is due in-plane vibration of sp^2 carbon atoms and is degenerated in longitudinal and transverse phonon modes. In comparison with the three other discussed peaks, it is the only first order process (involving 1-phonon) [67].
- **D+D"-peak (or G*)** at $\sim 2450 \text{ cm}^{-1}$: This peak is due to the association of a phonon from the D-peak and an acoustic phonon. In our analysis, it is useful to confirm the thickness of flake, that is first evaluate with the 2D-peak.
- **2D-peak (or G')** at $\sim 2680 \text{ cm}^{-1}$: This peak originates from two opposite wave vectors phonons that where momentum is conserved. Because there is no need for defects to activate them, they are thus always present. Looking at width of this peak is a key point to determine if the flake is a single or a double layer [68].

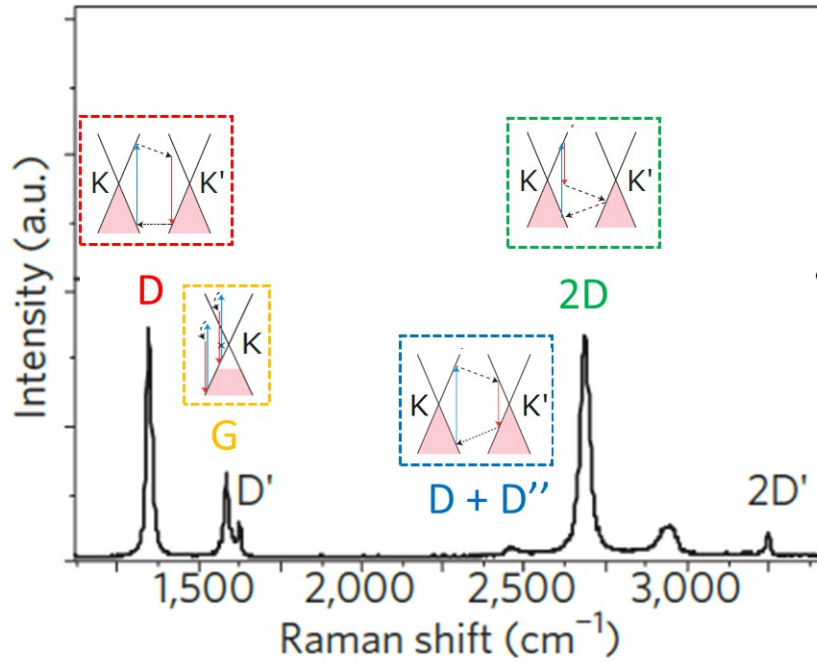


Figure 4.13: Typical spectrum of pristine graphene. The most insightful peaks, D, G, D+D'' and 2D are highlighted in colors. For each, the phonon transition process is represented from the electronic band near the Dirac cone of graphene. Blue arrows stand for phonon absorption and red arrows for phonon emission. The black dashed arrows represent the emitted phonons in the transitions. Adapted from [68].

Thickness resolution:

As mentioned in the previous section, the useful peaks for the thickness analysis are the D+D'' and especially the 2D. The whole spectrum graph and the 2D peak focus of Figure 4.14 will help the analysis. A first general comment is the increase of the G peak amplitude in comparison with the 2D peak while increasing the number of layers. It reaches a maximum at 9 layer graphene [67].

Then, the best tool to differentiate mono-layer from bi-layer is the shape of the 2D peak. In single-layer graphene, the peak is a symmetric sharp Lorentzian shape. However, in bi-layer graphene, the Lorentzian is offset to higher wavelengths, wider and and not symmetric anymore. This particular shape is in fact the convolution of four Lorentzian labeled as $2D_{1A}$, $2D_{1B}$, $2D_{2A}$, $2D_{2B}$. Those come from the interaction of the graphene planes that causes the π and π^* bands to divide in four. There are 4 possible combination of scatterings for the two opposite wavevector phonons involved. Each of these four transitions spawn a Lorentzian peak.

Finally, the D+D'' peak switches from a sharp peak in graphene, to a rounder and flatter peak for thicker flakes.

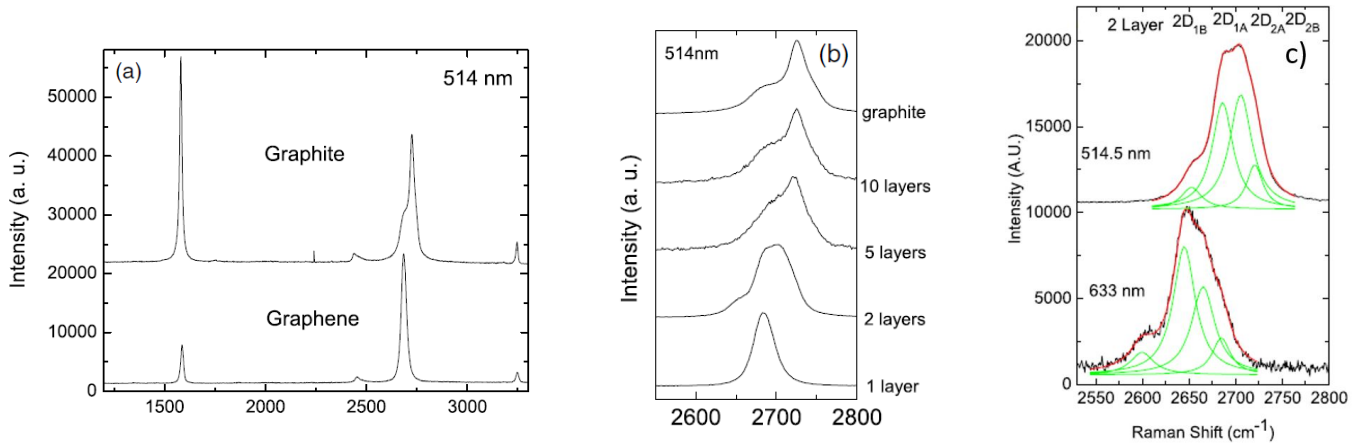


Figure 4.14: a) Raman spectrum for pristine graphene and graphite with a 514 nm laser. b) Evolution of the 2D peak for different amount of stacked graphene layers. c) Decomposition of the 2D peak of the bi-layer graphene in its four components both with a 514 nm and 633 nm laser. Adapted from [69].

Measurements:

On Figure 4.15 a), a graphene and graphite flake respectively highlighted in dotted green and red lines coming from an exfoliation batch. On Figure 4.15 b), the Raman spectrum performed on these two flakes in the laboratory.

The spectrum shows no D peak at $\sim 1350 \text{ cm}^{-1}$. This proves the absence of a significant amount of defects. Indeed, mechanical exfoliation of graphite by cleavage yield to very good quality graphene. As expected, the 2D peak is offsetted higher and is wider from the sharp peak of the mono-layer. Same observation for the D+D'' peak which is flatter. In addition, the G peak relative amplitude is bigger in the graphite.

The flake in Figure 4.10 gives the same spectrum signature as the flake of Figure 4.14. That is enough evidence to call it a mono-layer and use it to build the Hall bar for the experiment.

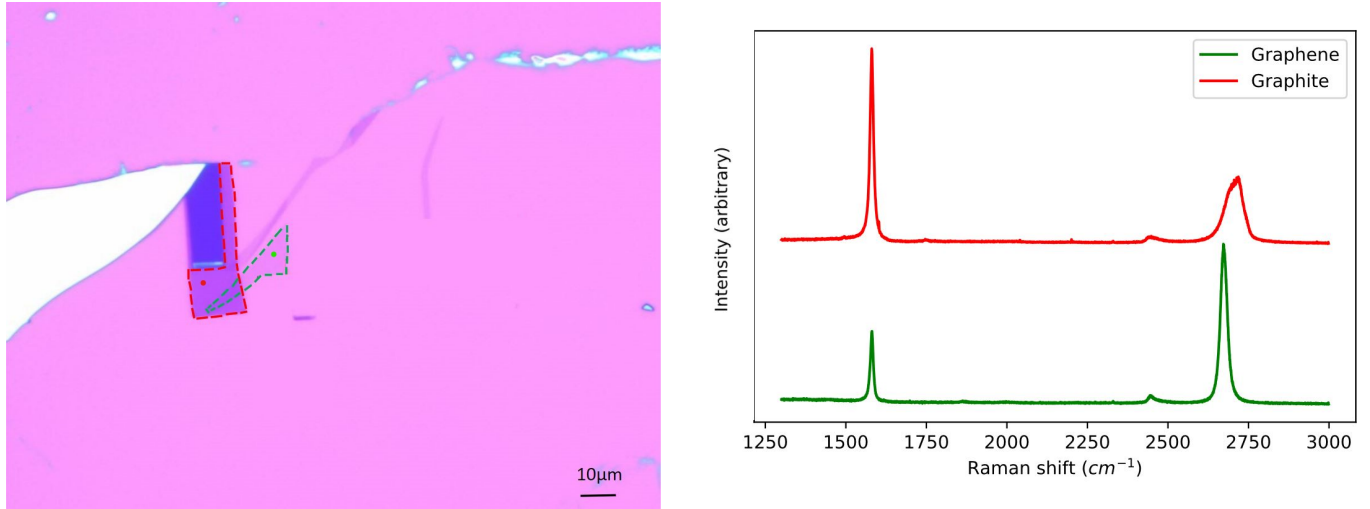


Figure 4.15: On the left: Optical microscope capture of a mono-layer flake highlighted in green dotted lines and a multi-layer flake highlighted in red dotted lines. The graphite overlaps the graphene on a portion of its area. For the spectroscopy, the laser is focused on the green dot or on the red dot. On the right: Raman spectrum from 1300 to 3000 cm^{-1} with corresponding colors to the highlighted areas.

4.5 BN under the microscope

Now that the candidate flake has been confirmed to be a single layer, it is the moment to select two appropriate BNs among the batch of exfoliation. The conditions under the boron nitride flakes are less constraining than those required for graphene. For instance, the thickness of the flake should not be a single plane. In fact, the ideal BN is not too thin but not too thick. If it is too thin, picking it up from the wafer is more delicate and if it is too thick. Satisfying thickness range from coloration between dark blue and turquoise.

Ideally, the graphene should fit between the layers of BN without exceeding the edges. In this particular case, the graphene flake measures more than 100 μm in length which is astonishingly long. Finding BN this size has been challenging. This is why a portion of the graphene will be lost in the picking process. Moreover, boron nitride surface should also be homogeneous and spaced from the edges of the wafer.

On Figure 4.16, these are the two candidates selected to encapsulate the graphene. They are wide enough but shorter than the graphene. Moreover, they are clean, homogeneous and far from the edges of the Si / SiO₂.

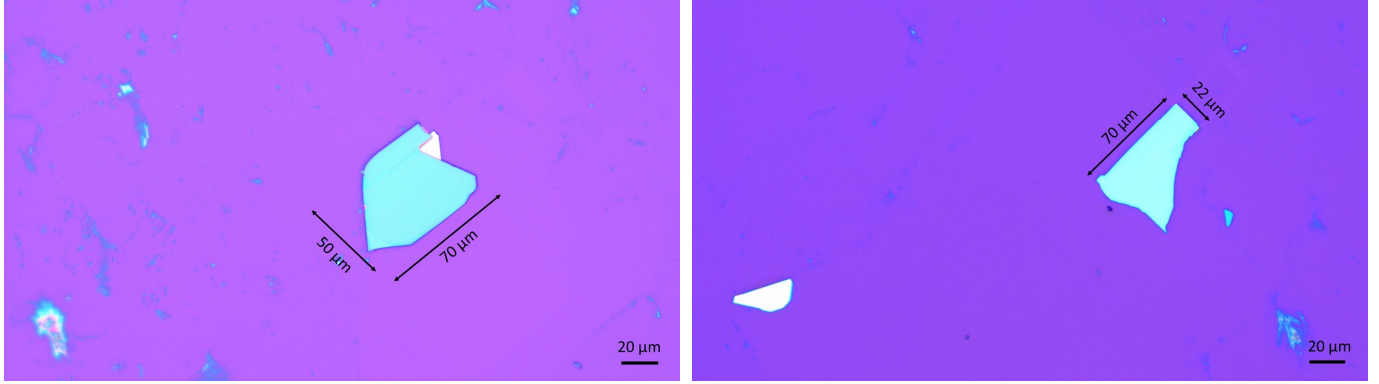


Figure 4.16: Optical microscope capture of intermediary thick BN flakes measured.

4.6 Transfer technique

This section is dedicated to the assembly of the heterostructure. As a reminder, the desired stack is a graphene layer encapsulated between multi-layers BN laid on a Si/SiO₂ wafer. Ideally, graphene would have been grown directly on the BN flake surface. However, it is still hypothetical to grow graphene on non-metallic substrates [70]. This is where the transfer process comes into play. It allows to stack different 2D crystals one by one.

Transfer processes take shape in different ways but can be classified in two categories: wet transfer and dry transfer.

4.6.1 Wet transfer

Wet transfer methods involve interaction between a liquid solution and the flake at some point of the process. An example of wet wedging technique is presented and detailed in Figure 4.17. While the flake being in contact with the solution, some contamination is still possible which might result in undesired doping. Also, it is not possible to obtain the relative positioning of one flake to another. Yet, in our experiment, a remarkable precision is needed for the stacking. Therefore, dry transfer techniques are preferred here.

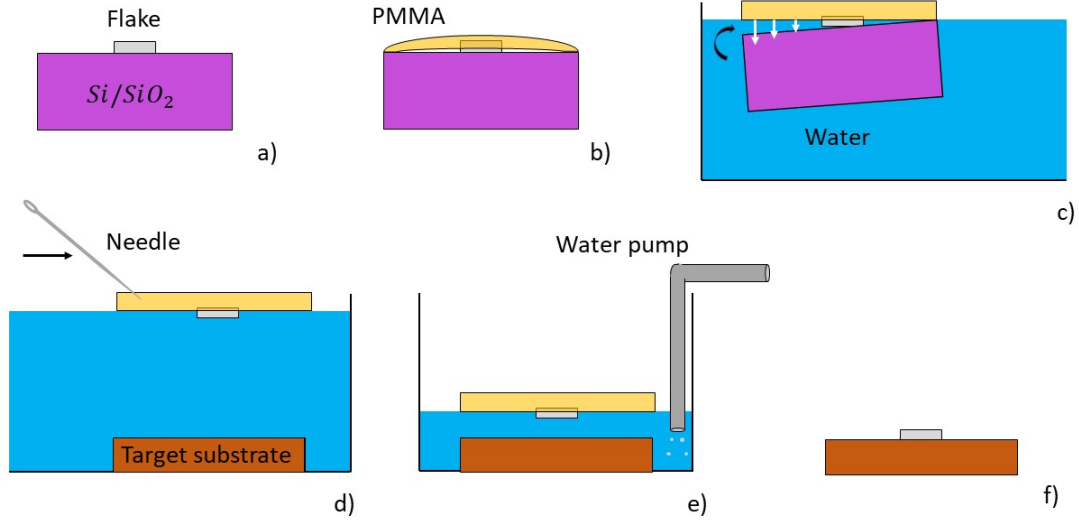


Figure 4.17: Wet transfer method called wedging transfer. a) The flake to be transferred is exfoliated onto a hydrophilic substrate such as Si/SiO₂. (b) The wafer with the flake is coated with a layer of PMMA which is a hydrophobic polymer. c) The stack is then immersed in H₂O where the water molecules can slide between the SiO₂ and the polymer until they are completely detached. The polymer film carrying the flake remains floating on the water surface. d) The target substrate for the transfer is also immersed. A needle coupled to a micromanipulator can be used to gently position the floating polymer above the substrate. e) The water of the container is pumped and the flake contact the substrate. f) The polymer is dissolved leaving the flake transferred onto the final substrate. Adapted from [71].

4.6.2 Dry transfer

Dry transfer methods are based on the intense vdW interaction between graphene and hBN. Indeed, this interaction is stronger than the interaction between graphene and substrate or hBN and substrate. This is what makes the stacking doable.

As for the wet-transfer, each dry transfer technique has its own subtleties. For instance, the choice of polymer may vary, the temperature for the contact or even the substrate to transfer the tape of exfoliation [71]. However, the global process stays the same. In the context of this work, the method of ref [72] is followed.

Transfer slide:

The first step is to build what will act like a fishing rod for picking up flakes: a transfer slide. To peel off a flake from the Si/SiO₂, a sticky film polymer is used: polypropylene carbonate (PPC). But, the process is not as easy as simply laying down the 2D surface of the PPC on the flake and then lifting it up. If the PPC is embossed, the control on the contact surface with the wafer is superior. This leads to a smooth application of the force between PPC and the wafer. Furthermore, if the polymer exhibits no relief, chances are high to collect other valuable flakes, and that would be a waste.

To overstep this issue, a small cubic piece of soft polymer is placed first on the glass slide. Polydimethyl siloxane (PDMS) is often used because of its transparency and softness. The alignment with the substrate is done by an optical microscope going through the slide. Thus, PDMS has to be flat and homogeneous. It is fixed to the slide with the transparent tape mentioned in the exfoliation process. Meanwhile, two or three drops of a 15-85% PPC diluted in anisole are applied on a cleaned 1x1 cm Si/SiO₂ wafer. Afterwards, it is spin-coated at 2000 rpm for a minute. The PPC should be spread uniformly. Then, the anisole is evaporated by heating the wafer at 110° C for about 10 minutes. PPC is ready to be placed on the PDMS. Firstly, it needs to be collected. A way to achieve it is to punch a hole in a piece of tape and drop it off on the PPC. When the tape is peeled off, a circular PPC layer should fulfill the hole. All that remains is to center that layer on the PDMS and heat up the whole at 110° C. This temperature (higher than PPC glass transition) ensures the PPC to be smooth and flat before the picking.

A schematic representation of the process is presented in Figure 4.18 and 4.19.

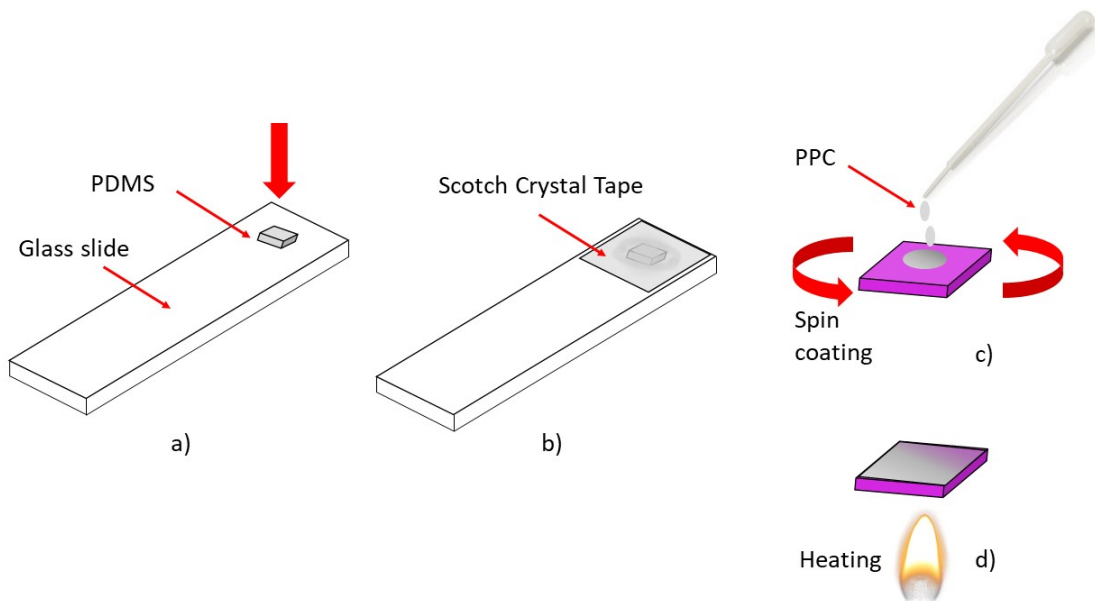


Figure 4.18: Preparation of the transfer slide for dry transfer. (a) a cubic piece of $\sim 1.5 \times 1.5 \times 1.5$ mm of PDMS is cut and laid down on a glass slide. (b) The PDMS is stuck to the slide by a transparent Scotch Crystal tape in order to form a bumpy shape. (c) A cleaned Si/SiO₂ wafer is spin-coated by a PPC layer dissolved in anisole. (d) Then, the wafer is heated to evaporate the anisole.

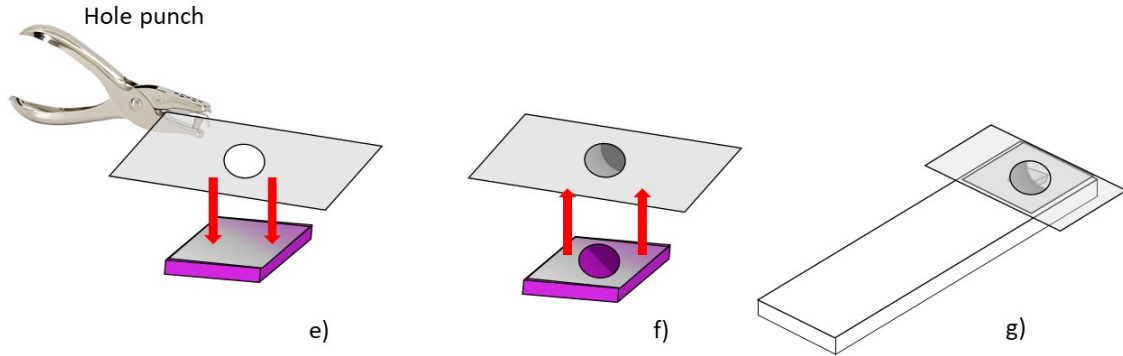


Figure 4.19: Follow up of the preparation of the transfer slide for dry transfer. (e) A hole of ~ 1 cm diameter is punched in a piece of sticky scotch tape. This tape is laid down on the wafer surface. (f) Then, the tape is peeled off carefully and the hole should be filled with a layer of PPC. (g) This piece of tape is stuck on the bumpy PDMS of the glass slide.

Transfer setup:

To realize the pick up or the release of a flake, several parameters have to be gathered: a perfect alignment on the substrate, an excellent control on the contact point and a regulation on the temperature. In this sense, the glass slide is set up on a transfer table. This transfer table is assembled with micrometer screws and a temperature controller. There are in total six screws: three governing the movement of the glass slide in the xyz plane and three for the wafer in polar coordinates $xy\theta$. Using the θ screw allow to rotate the wafer against the glass slide for a perfect alignment.

It is also essential for the wafer to stay still when pressure is applied with the glass slide. For this purpose, the wafer is standing on a small hole in the Aluminum which is connected to a vacuum pump. This way, the wafer maintained firmly. Under the wafer holder is hidden the Peltier cooler/heater. Aluminum demonstrates low density and pretty high thermal conductivity allowing heat to flow quickly to the wafer. As Peltier effect depends on the ΔT between two points, the copper stage below is a heat reservoir and keeps a constant temperature thanks to the water tank connected. Thus, a PID controller can access the relative temperature of the aluminum and regulate the voltage in the Peltier cell.

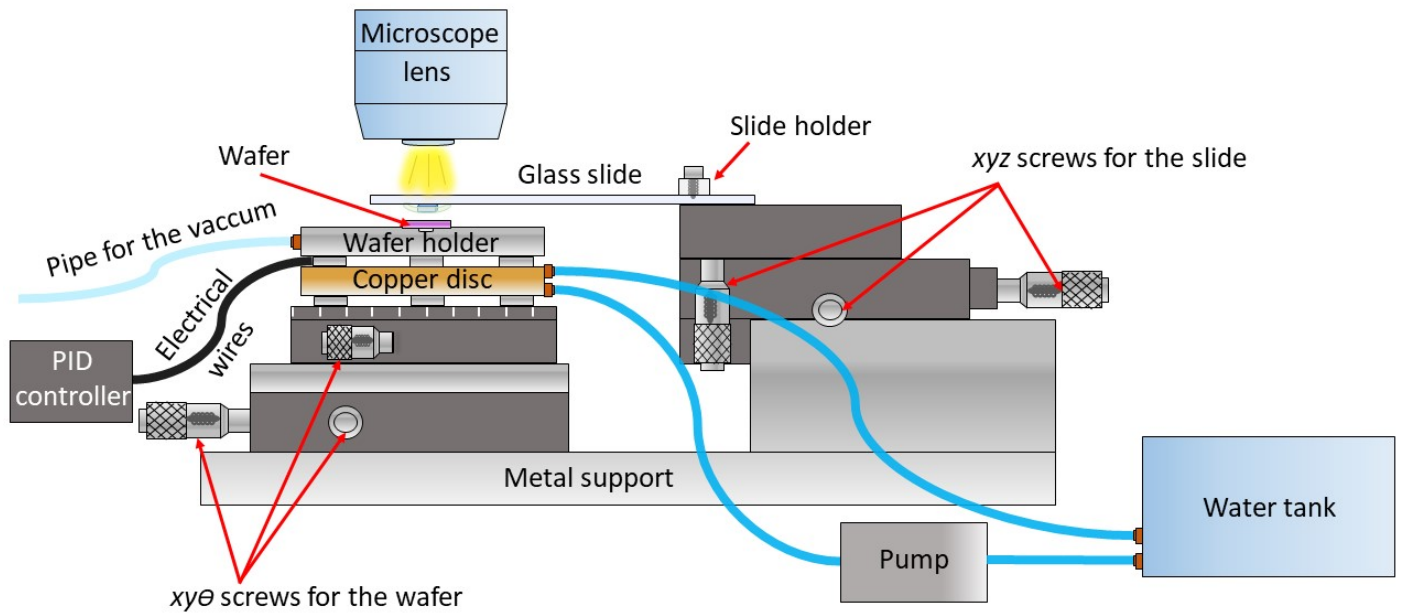


Figure 4.20: Dry transfer table with a glass slide mounted under an optical microscope.

Transfer process:

When the Si/SiO₂ wafer is held on the Aluminum stage thanks to the vacuum and the glass slide is properly screwed, the picking process can start. The PPC bump is roughly placed over the wafer. With the help of the optical microscope, the flake of interest is aligned below the transparent PDMS cube. A clean and flat area of PPC has to be chosen to interact with the flake. Indeed, whereas the PPC has been heated, dust or small bubble can still alter its functioning. Then, the transfer slide is gently screwed down toward the wafer. Ideally, the first contact area with the wafer is not directly on the flake but quite close. The contact is visible by a change of color of the background and a bi-color contact front appear (Figure 4.21 b)).

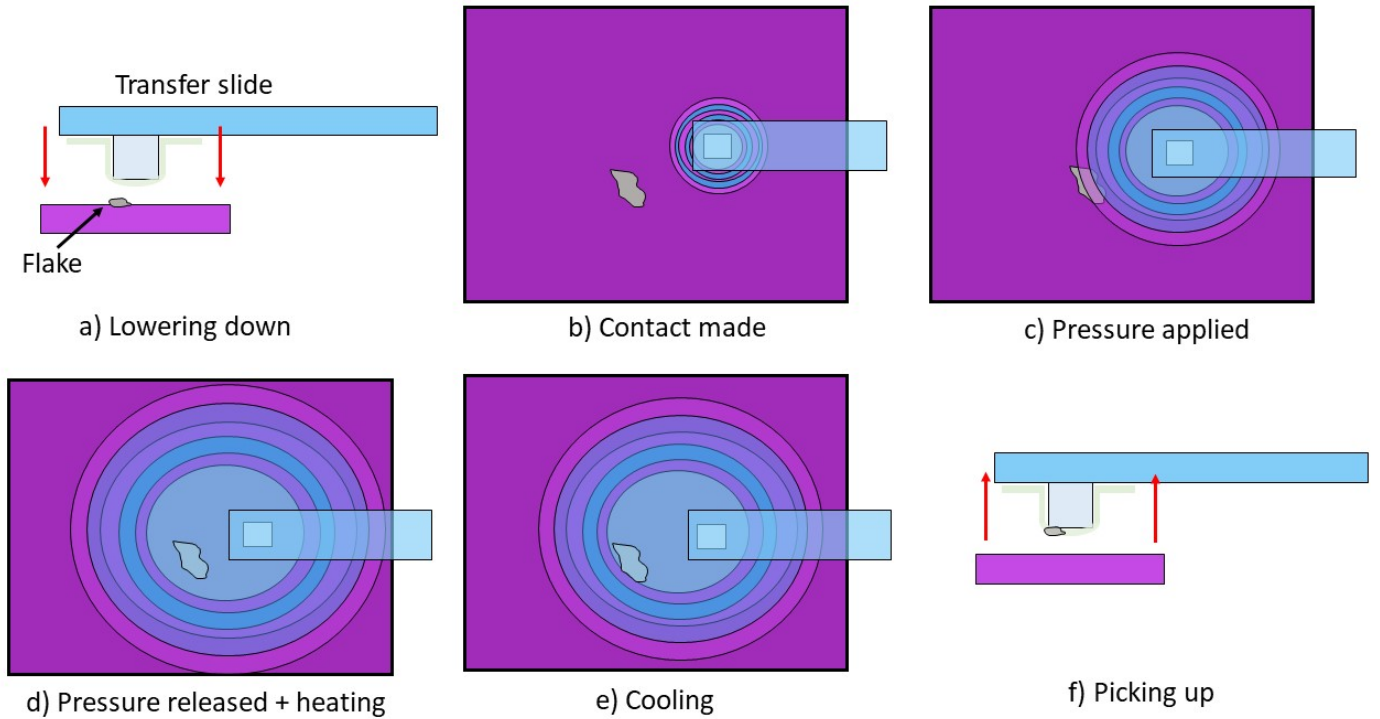


Figure 4.21: Process of picking up a flake from Si/SiO₂ with the transfer slide.

As the PPC has a bumpy shape, lowering it more and more increases progressively the circular contact area. The lowering should stop when the contact front is about to swallow the flake (Figure 4.21 c)). At this moment, the heating take over. Indeed, increasing the temperature up to 50° C will make the PPC and its contact front spread on the wafer. This step is essential for the PPC to flow smoothly on the flake. The heating should be stop when the contact front has overshoot the flake. It could take seconds to minutes depending on the size of the material to pick up. Now that PPC is homogeneously spread over the flake, the temperature is lowered down to 5° C. This temperature is way below the glass transition of the PPC and allows to fixed firmly the flake on it. One should be careful not to drop the temperature below 0° C in order to avoid water condensation on the wafer. During the cooling, the contact front might retract. It is not an issue as long as the front does not step over the flake. Once the 5° C is reached, one tries to maintain this temperature for about a minute. Then, the PID is let free to come back to room temperature. The contact front will shrink during this operation. With the screw that maintains the glass slide, it is crucial to control the speed of uplift. Indeed, with the temperature increase, the PPC might "unglue" of the substrate very quickly. From experience, successful pick ups have been realized by maintaining a slow speed of lift up.

If the flake becomes white when the glass slide is lifted up (Figure 4.22 c)), it has been the transfer is a success. Otherwise the process of heating and cooling need to be restarted.

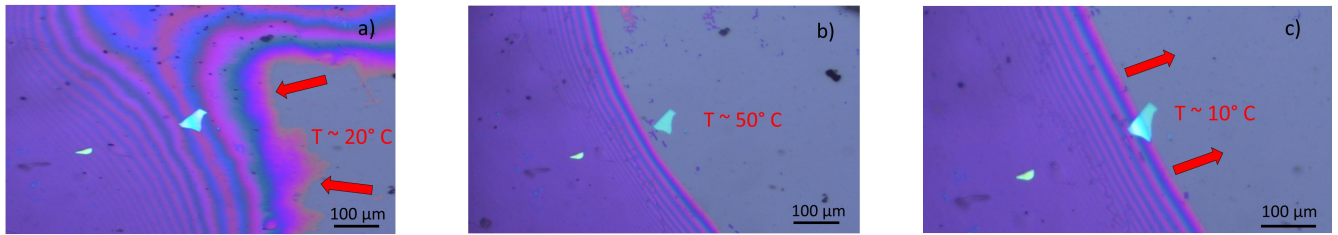


Figure 4.22: Microscope images of the transfer steps to collect a BN flake. (a) The contact area is next to the flake. Screwing down the transfer slide make the contact front spreading across the substrate. (b) When the contact front is about to overlap the flake, temperature is raised up to 50° C and the contact front keep on going. (c) Temperature is raising from 5° C to room temperature. The flake is changing color to a bright white when the contact front is overlapping it.

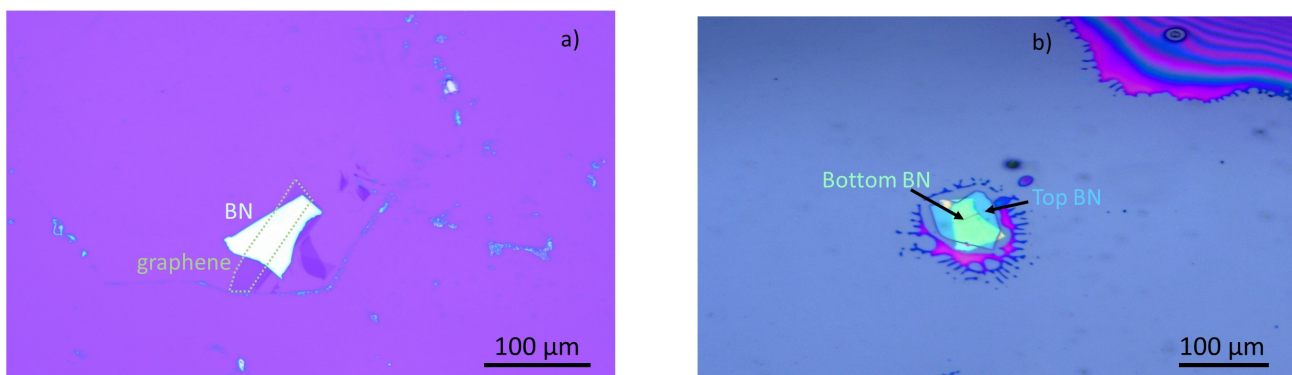
Stacking process:

Of course, there is a sequence to follow to build the stack. First, a BN flake. Then the graphene flake. Finally the second BN flake. Lets assume that the first BN flake has been collected on the PPC. The follow-up of the process is the same with one exception: BN and graphene have to be perfectly aligned and superimpose themselves during the lowering of the glass slide. By changing the focus of the microscope, it is possible to center the boron nitride flake of the PPC on the graphene of the wafer.

This time, it is the higher strength of the vdW forces that will "unglue" the graphene of its interaction with the substrate. There are also conditions on the choice of the first BN to pick. Indeed, it should be the one between the two BN to be the closer size and shape in comparison with the graphene flake (Figure 4.23 a)). To explain this, let's recall that BN is quite thick and not as transparent as graphene is. Thus, when the first BN and graphene are stacked, the graphene is being hidden. It is no more visible. So, if the first BN picked up is way larger than graphene, there might be issues of alignment between the graphene and the second BN. This is the reason why the first boron nitride should be smaller than the second.

Once the heterostructure is finished, a last pick up with the transfer slide is necessary to lay down the stack on a gold-marked Si/SiO₂ wafer (Figure 4.23 c)). These marks are a grid-pattern that allows to locate the stack with x and y coordinates. It will be useful in the following AFM and lithography experiments.

Finally, the heterostructure spends two hours in a RTA oven at 350° C to evaporate as much stuck PPC as possible.



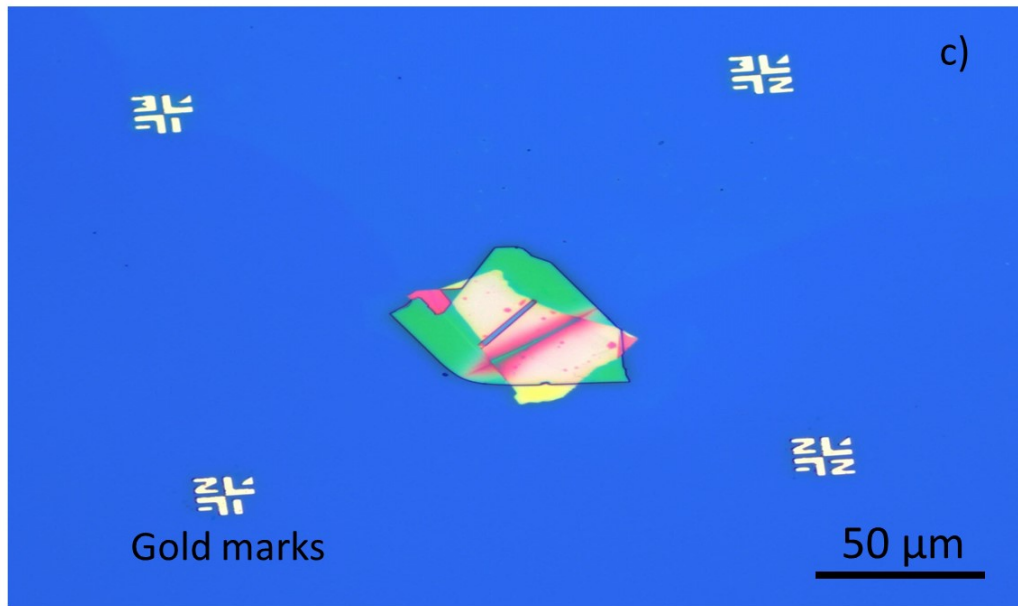


Figure 4.23: Microscope capture of the progress of the heterostructure. (a) BN laid down on graphene. This beginning of stack has to be picked up and dropped on the second BN. (b) The three-part stack under the PPC to be transferred to the marked wafer. (c) Completed stack on the gold-marked Si/SiO₂.

4.7 AFM imaging

The stacking process can be arduous and require repetition of the steps again and again to pick up flakes with success. Because of that, BN will have tendency to crease and form wrinkles (i.e. the two green transverse lines in Figure 4.23 c)). Furthermore, impurities such as remaining PPC can sit in the stack. Indeed, these factors can deteriorate the electrical properties of the graphene.

AFM imaging is a great tool to get a clearer global view of the stack. The topography and the thickness of the sample can be measured in the tapping mode.

The AFM is composed of a cantilever that can oscillate at its resonant frequency. At the very end of this cantilever is a small tip. Positioned close to a sample, the apex of the tip interacts with the atoms of the surface. These forces have different origins: vdW forces, electrostatic forces, dipole-dipole, ... Meanwhile, a laser is focused on the backside of the cantilever and its reflection is captured on a 4-quadrant photo diode. This photo detector is connected to a feedback loop that control a piezoelectric element modifying the cantilever height.

Tapping mode:

In tapping mode, the tip of the cantilever is freely oscillating at its resonance frequency with a specific amplitude. This oscillation is achieved thanks to a piezoelectric material connected to the cantilever holder. To analyze the topography of a material, the cantilever scans the entire surface. When the tip is brought closer to the sample, the amplitude and frequency of the tapping oscillation is modified. This variation is also visible on the position of the deflected laser on the photo diode quadrants. Converted, this signal gives the relative height of the sample on a precise area. While

scanning, the relative height of the cantilever is adjusted to maintain the set oscillation amplitude. Figure 4.24 shows the set up used in tapping mode for the surface mapping of the stack.

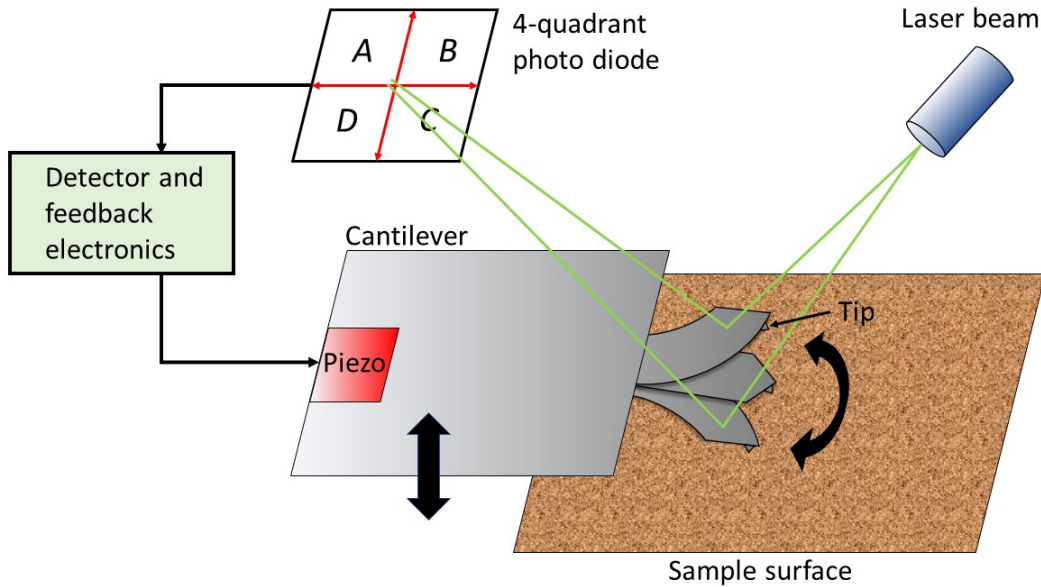


Figure 4.24: Schematic representation of a typical configuration of a AFM in tapping mode.

Results:

On Figure 4.25, the presumed wrinkles on BN layers are confirmed. The wider one is shaped like a step and the other is a smoother peak. The distance between these two wrinkles is about $15 \mu\text{m}$. The decision was taken to use the flat areas on the left and right of these steep layer hills. A side for the simple constriction bar and the other side for the double constriction bar, thanks to the considerable length of the graphene. The Figure 4.26 allows to better visualize the area to avoid and the ones that will later be etched. On the sides, the usable area is also limited to the places where BN superimpose for a complete encapsulation.

On the right of Figure 4.27, the cross-section profile on the length of the stack is represented. The stack is about $150 \mu\text{m}$ thick with peaks of an additional $100 \mu\text{m}$.

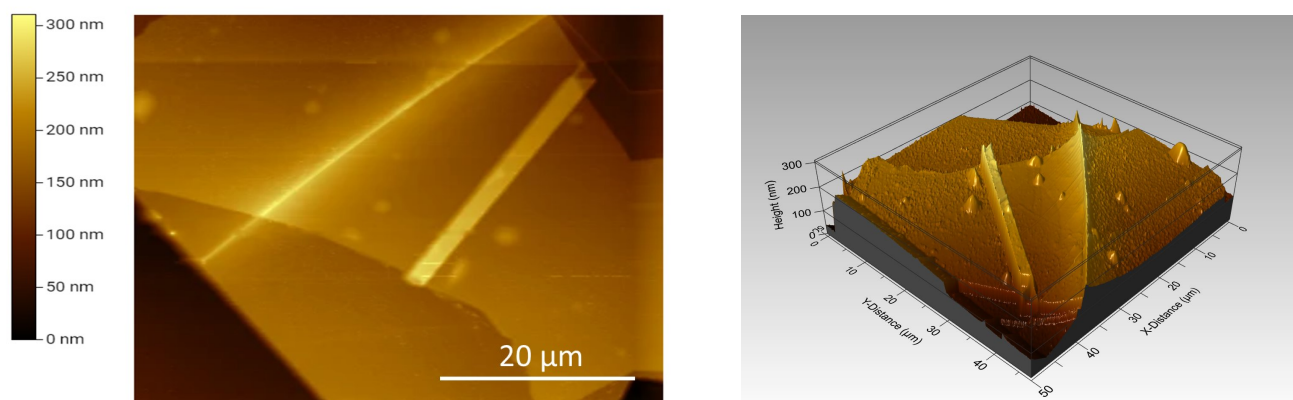


Figure 4.25: On the left: tapping AFM image of the stack. On the right: 3D image of the topography of the stack.

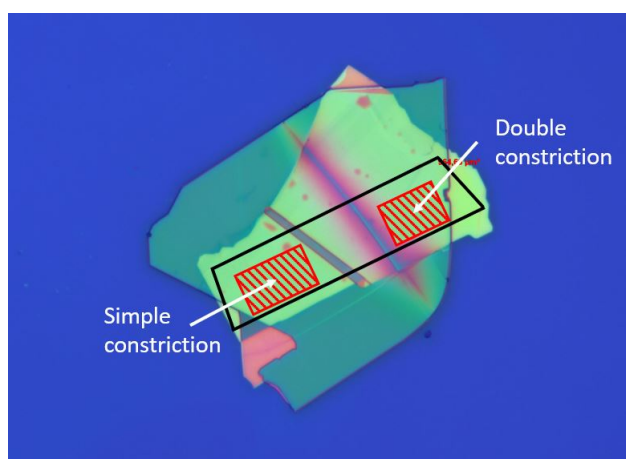


Figure 4.26: Representation of the hatched areas where the single and double constrictions will be designed. The black trapeze shape represents the approximate location of the flake of graphene beneath the BN layers.

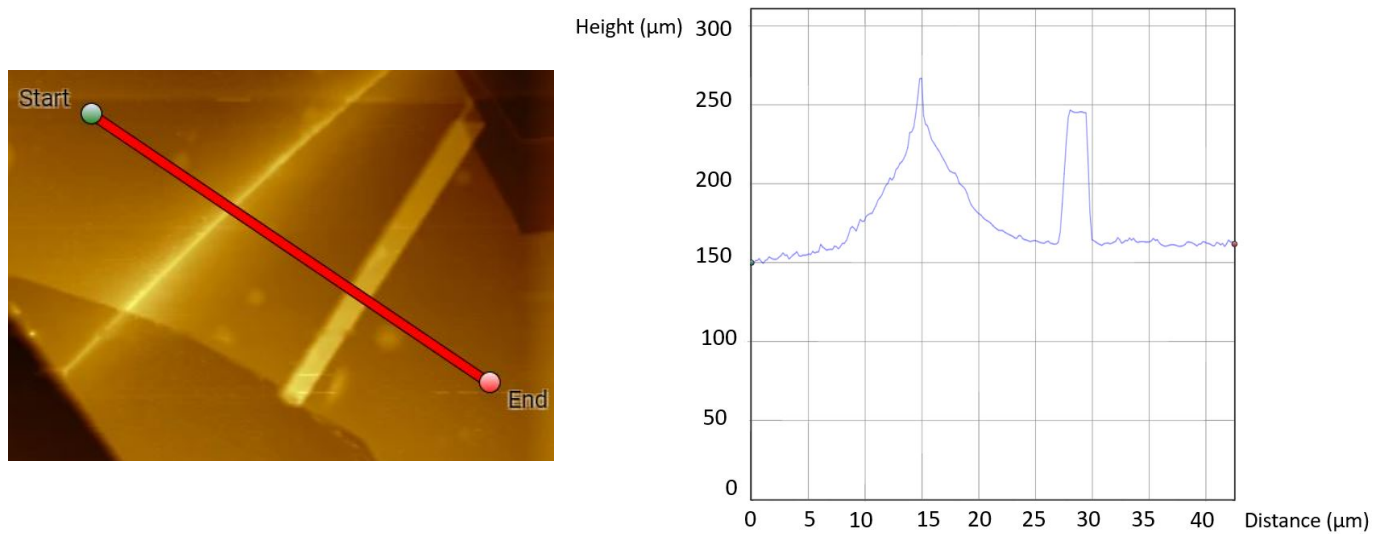


Figure 4.27: Cross-section profile computed from the green dot to the red dot.

4.8 Last steps of fabrication

The fabrication process had to be stopped in the Winfab laboratory as the electron-beam lithography could not be performed. Thus, the last steps of fabrication have been made in the laboratory of the Université de Paris. In this section, a brief review of the remaining procedure is described.

Hall bar shaping

The first step is to design the single and double constriction with the available space. These designs with the paths of metallic leads are sketched with Klayout (see Supplementary section) for the lithography file used). Gold marks on the wafer allow to locate and map precisely the stack for the sketch. Once the design is done, the procedure can start. The stack is spin-coated with a polymer sensitive to radiations (often PMMA); it will serve as a resist. Then, the PMMA is baked to remove the excess solvent and to dry it. At this stage, the stack is ready to be exposed under the electron beam. As the PMMA is used as a positive resist, the outline of Hall bar has to be bombarded. Electrons tend to weaken or break the chemical bonds of the polymer. After the exposure, the sample is immersed in MIBK solvent for a minute and a half. Only the exposed PMMA is dissolving. Then, the remaining MIBK is rinsed with isopropanol and dried thereafter. What is left is a Hall bar shape with the constriction protected under PMMA. Then, the stack is exposed to O_2 plasma that will produce very anisotropic profiles. With the right parameters, the graphene-BN sandwich is totally removed in the unprotected areas while on the Hall bar, only a part of the total PMMA thickness is etched away (generally about 100 nm).

Contacting

The next step is to contact the leads of the bar. Indeed, for electrical measurements, one needs to connect macroscopic pins to the leads by bonding. To this end, larger metallic paths ended with a

metallic pad (few hundreds of micrometers sides) are used to spread apart the leads on the surface of the wafer. They must be visible with an optical microscope used in the bonding process. Those metallic paths are created once again with a lithography technique. The wafer is spin-coated with the PMMA. This time, it serves as a sacrificial layer. Areas where the contacts paths will be patterned are exposed under the e-beam lithography and then developed with MIBK. The paths carved out of PMMA are ready for metallization. Electron beam physical vapor disposition (EBPVD) of Au/Ti is often used for this purpose. Finally, the sample is immersed in acetone to remove the remaining PMMA and the undesired gold is removed by lift-off.

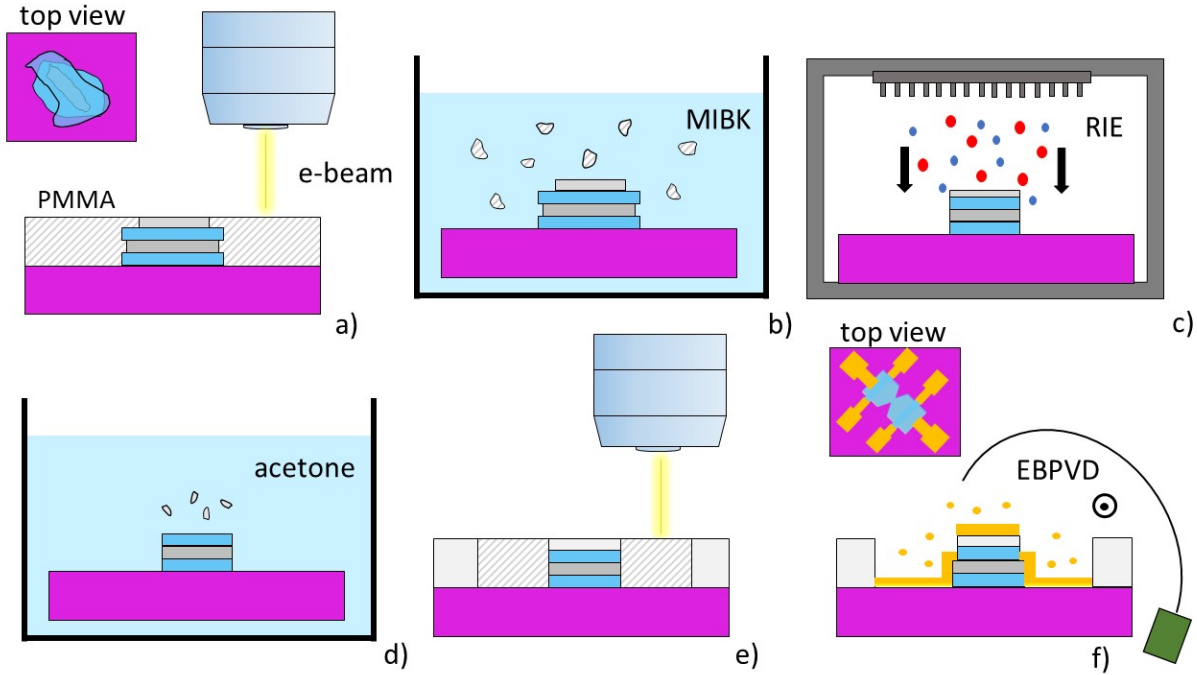


Figure 4.28: General view of the last steps of the fabrication process: (a) E-beam lithography of the sample covered in PMMA. (b) Dissolution of the exposed PMMA in MIBK. (c) Reactive ion etching to shape the Hall bar. (d) Dissolution of the remaining PMMA. (e) Further lithography to create the metallic paths. Once again, dissolution in MIBK. (f) Electron-beam physical vapor deposition followed by dissolution of the PMMA and lift-off of the undesired gold layer.

4.9 Electrical measurements

To test if current pass through our samples it is needed to built a setup allowing to connect electrical cables between the sample and the measurement devices. It is a lock-in amplifier used for measurements in the low and medium frequency range. The first step of fabrication was to place the sample on a specimen holder adapted for the lock-in (Figure 4.30). The specimen holder (Figure 4.29) is constituted of a central rectangle in which the sample is placed and of long electrical pins situated on both sides. These pins are linked to smaller pins situated on the fourth sides of the central square. So for one big pin it corresponds one smaller pin. It will be very useful for the next steps.



Figure 4.29: Specimen holder constituted of 40 small metallic pins connected to 40 larger ones.

After that, it was needed to make a bounding to join each metallization pads of the sample to electrical pins of the specimen holder. It is denoted by bonding contacts on the following figure. The next step is to place the all setup on a allowing to connect the specimen holder to the MFLI. Knowing the correspondence between each pads and pins, it is possible to choose both pins between which the current will flow [73].

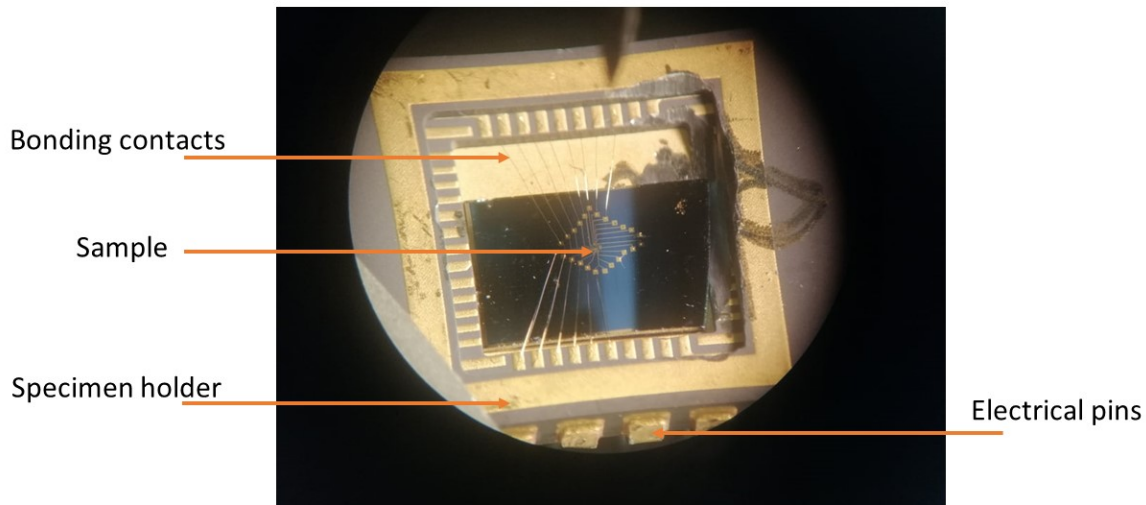


Figure 4.30: Capture of the wafer welded in the specimen holder. Each of the metallization pads is connected to pin.

After testing all possible couples of pins, it turns out that in both samples no current was flowing.

Astonishingly, it is even the case between two adjacent pins. Here are some hypothesis made to explain this disappointment:

- A first explanation could be the fact that the constriction cut the sample. The lithography is not flawlessly perfect. Even if a marge of error was take into account, it is still possible that the lithography cut the sample in two at the constriction.
- A second hypothesis is the precision of the positioning of graphene under the flake of BN. Indeed, during the drawing of the lithography sketch, it was arduous to determine with precision the relative position of graphene according to the BN. A slight shift could generate a mistake during the etching process and therefore leads to parts of the Hall bar with no graphene.

Chapter 5

InGaAs/InAlAs electronic interferometer

The following section is based on a draft of paper called *Transition from Coulomb Diamonds to Checkerboard-like Spectroscopies in Mesoscopic Quantum Hall Islands* by S. Faniel et al. It deals with the experimental measurements of magnetoresistance and SGM data in an InGaAs/InAlAs QPC allowing the transport in a 2DEG. It highlights oscillations for different filling factors ν . These resistive interferences are explained by the tunneling of electrons between counter-propagating edge states on opposite sides using a QHI as intermediate. The QHI is not generated by an SGM tip but is of disorder-induced origin. The goal of this paper is to demonstrate similarities with objectives of this work. Indeed, the basic elements are the same. In both works, the starting point is a Hall bar in the QHE regime with a constriction and artificial potentials. Then, it could be interesting to compare and reproduce some results of this paper and try to reproduce their experiments in simulation with Kwant.

5.1 Parameters and results of the paper

The sample introduced in the article is made from an $\text{In}_{0.7}\text{Ga}_{0.3}\text{As}/\text{In}_{0.52}\text{Al}_{0.48}\text{As}$ quantum well. The 2DEG has a bare electronic density $N_s = 5.7 \times 10^{15} \text{m}^{-2}$ and a mobility $\mu = 5.3 \text{ m}^2/\text{Vs}$. Two trenches were etched with a constriction of 350 nm and the area beyond etched channels plays the role of side gate to manage the opening of the constriction. A schematic representation of the sample is shown on Figure [5.1](#).

All the transport measurements were performed with a magnetic field B perpendicular to the 2DEG and at a temperature of 100 mK . The graph [5.2](#) is the first experimental result for a side gate voltage $V_g = 5 \text{ V}$.

The figure shows high resistance oscillations like Shubnikov de Haas oscillations and small oscillations corresponding to AB effect. It was explained by the interaction between the counter-propagating quantum Hall edge channels in the mesoscopic system. A zoom on $\nu = 4$ was performed (the orange box of the graph [5.2](#) corresponds to the Figure [5.3](#)) to highlight different regimes when B is raised.

One can observe that B magnitudes between 5.2 T and 5.6 T corresponds to small oscillations around a plateau at zero resistance. Naturally, it is because all four edge channels at stake are transmitted through the QPC. QHI is surrounded by channel as represented in the inset I of Figure [5.3](#). By tunneling, edge states can backscatter leading to a raise of resistance which explains the oscillations

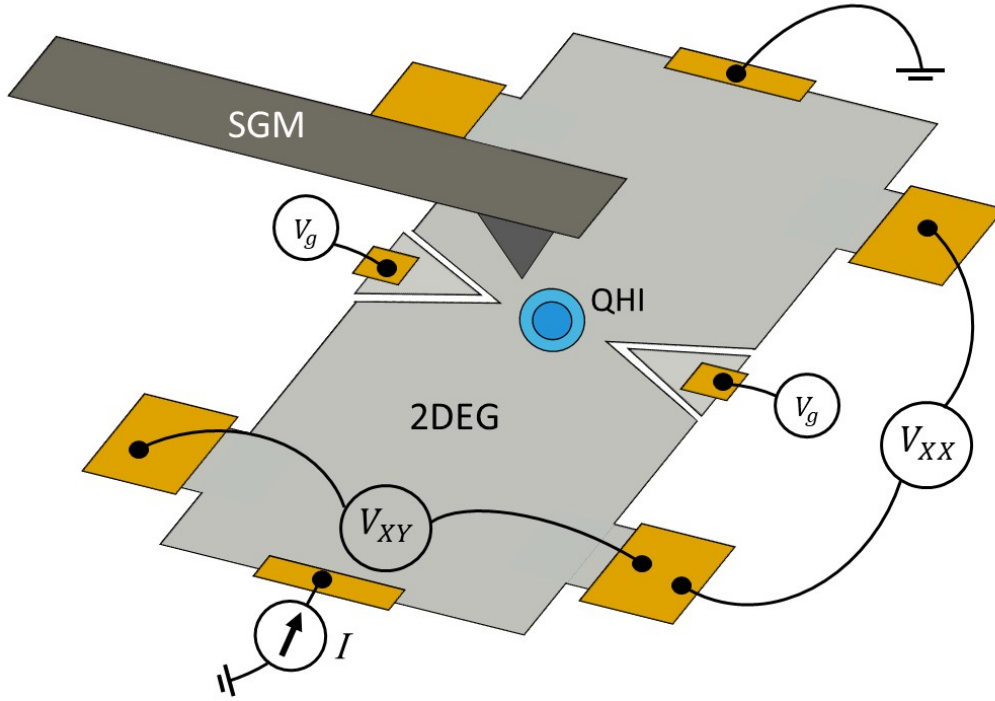


Figure 5.1: Representation of the experimental Hall bar. V_g is the tension applied in the trenches as side gates. The SGM scan the surface to locate the QHI represented in blue.

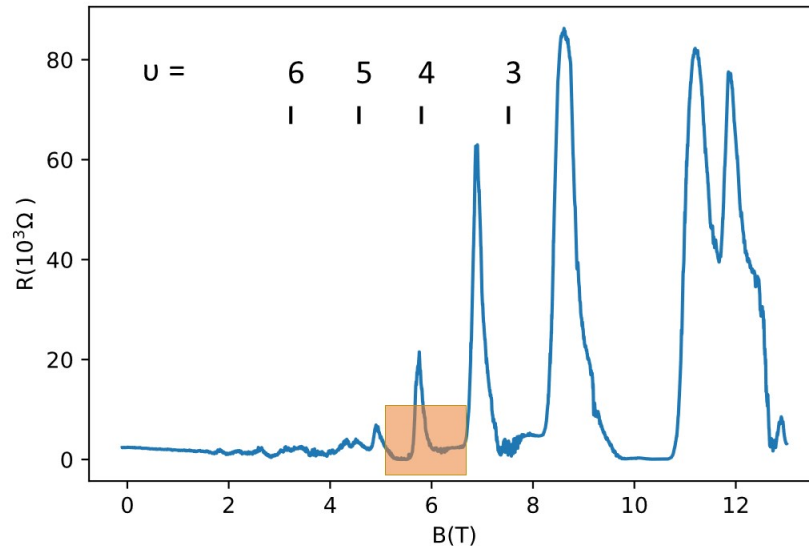


Figure 5.2: Experimental result for R_{xx} as a function of the magnetic field magnitude.

around zero. For a magnetic field between 5.6 T and 6 T a peak of resistance is observed. Indeed the Fermi energy crosses the highest Landau level and electrons can backscatter between counter-propagating edge states. Afterwards, when B is in the range of 6 T to 6.4 T , there is emergence of a plateau at around $2300\ \Omega$. Indeed, the number of states in the bulk ($N = 4$) is different than in the

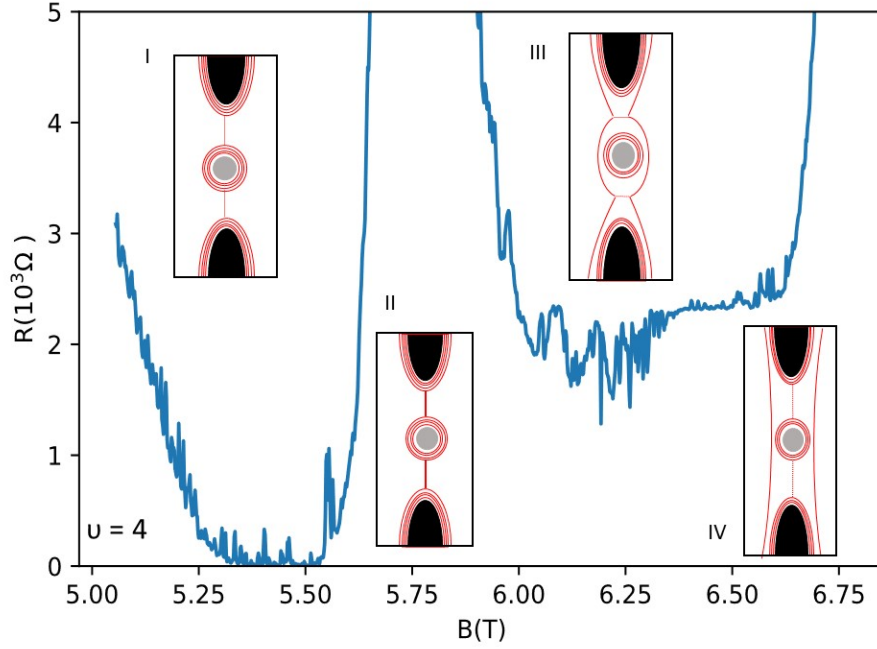


Figure 5.3: Experimental result for R_{xx} as a function of the magnetic field magnitude between $B = [5; 6.75]$ T at filling factor $\nu = 4$.

QPC ($N^* = 3$). The resistance can be computed via:

$$R = \frac{h}{e^2} \left(\frac{1}{N^*} - \frac{1}{N} \right) = 2151 \Omega \quad (5.1)$$

with e the electron charge and h the Planck constant.

Finally, for larger value of B , the resistance increases and creates another high peak. Indeed, as shown in the inset IV, the edge channel $n = 4$ is directly expelled and do not contribute anymore to the longitudinal transport.

The next part of the paper is focused on $\nu = 3$ of the graph 5.2. This range of magnetic field magnitudes is represented on Figure 5.4. In the blue box, there are oscillations under a plateau of 4300Ω . It is due to the reflection of one of the edge states in the QPC. It is similar to the configuration III in the previous graph with ($N = 3$, $N^* = 2$) leading to two edge channels transmitted through the QPC and the third one being coupled with the QHI forming an interferometer.

The figure 5.5 represents the differential resistance for $\nu = 3$ as function of the dc excitation voltage V and B . It highlights two regimes: one between 7.5 T and 7.56 T with a Coulomb diamonds pattern and one between 7.64 T and 7.7 T with a checkerboard pattern.

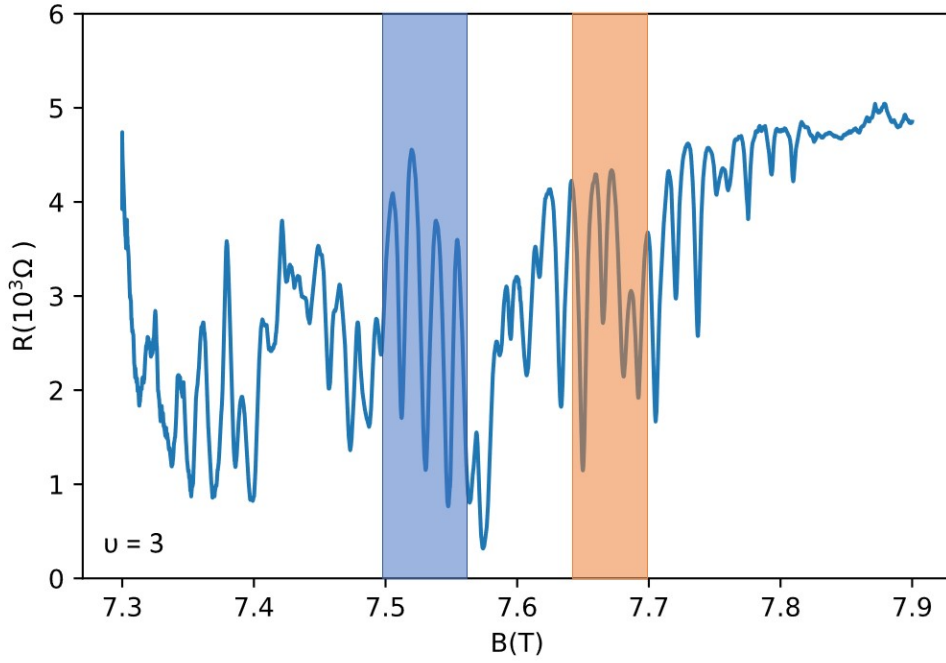


Figure 5.4: Experimental result for R_{xx} as a function of the magnetic field magnitude between $B = [7.3; 7.9]$ T at filling factor $\nu = 3$.

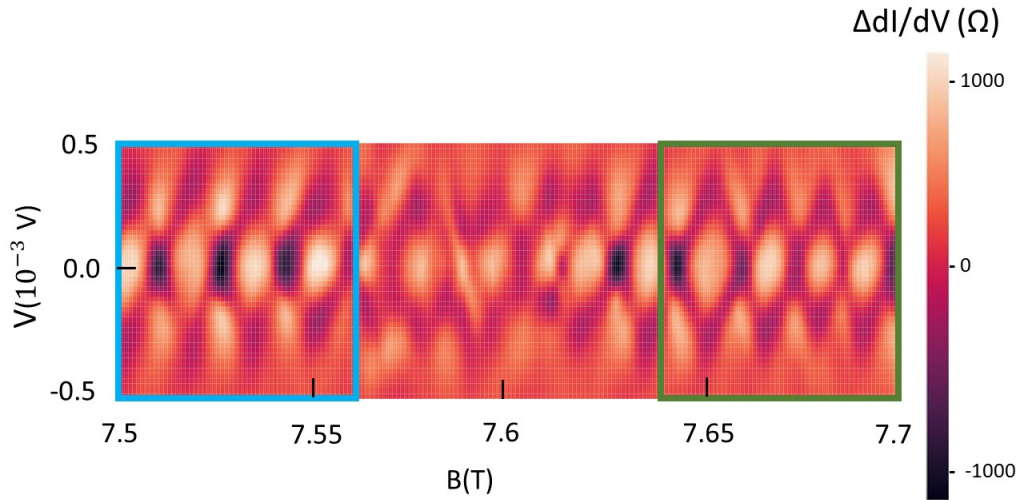


Figure 5.5: Resistance dI/dV as a function of magnetic field

5.2 Reproduction of similar results with Kwant

A similar sample can be simulated with Kwant to explain and reproduce the graph introduced above. A simple Hall bar of 500 nm width and 700 nm length with a square lattice and a potential at the center is built as shown here after on the heat diagram (Figure 5.6). The potential is the addition of two Gaussian shape function (one with a positive amplitude and one with a negative amplitude)

allowing to have the following heat diagram [5.6](#) and energy bands [5.7](#):

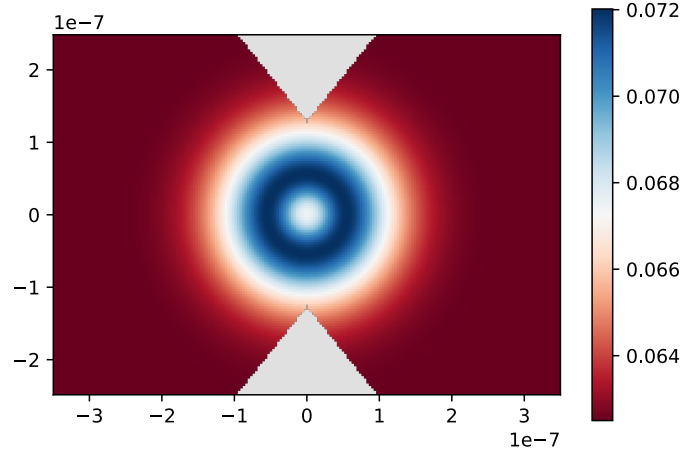


Figure 5.6: Heat diagram corresponding to a similar central potential than in the experimental results. It is 'donut' like shape allowing to have a different number in the bulk and in the QPC.

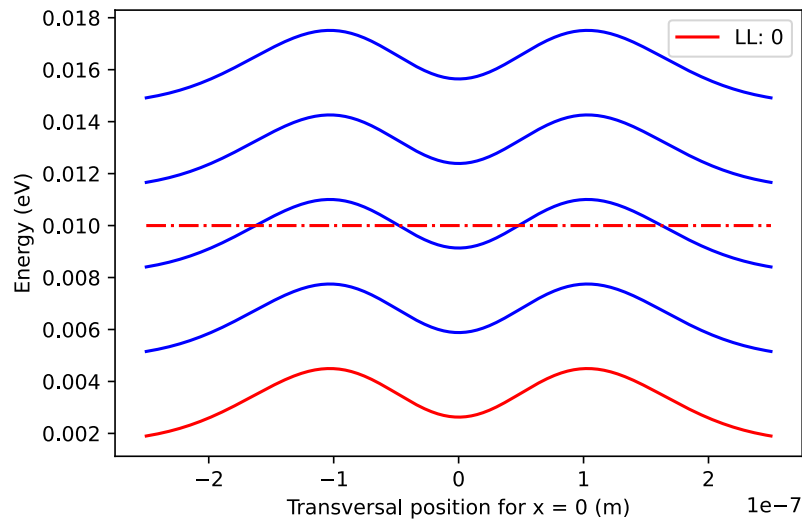


Figure 5.7: Energy bands in a transversal cross section for $x=0$. The Fermi energy is represented in a red dotted line.

To obtain the previous diagrams the following parameters were needed:

- Scaling $s = 8$
- Fermi energy $E_F = 0.01$ eV
- $V_{tip,1} = 0.014$ eV
- Standard deviation along x of the first Gaussian: $\sigma_{x,1} = 8.10^{-8}$
- Standard deviation along y of the first Gaussian: $\sigma_{y,1} = 9.10^{-8}$

- $V_{tip,2} = -0.01$ eV
- Standard deviation along x of the second Gaussian: $\sigma_{x,2} = 6.10^{-8}$
- Standard deviation along y of the second Gaussian: $\sigma_{y,2} = 7.10^{-8}$

It is now possible to obtain a comparable graph of the Figure 5.3 by computing the longitudinal resistance according to the magnetic field. The result is presented on Figure 5.8. One can observe multiple peaks but the most interesting thing is to highlight the plateau resistance as found in Figure 5.3 between 6 and 6.75 T.

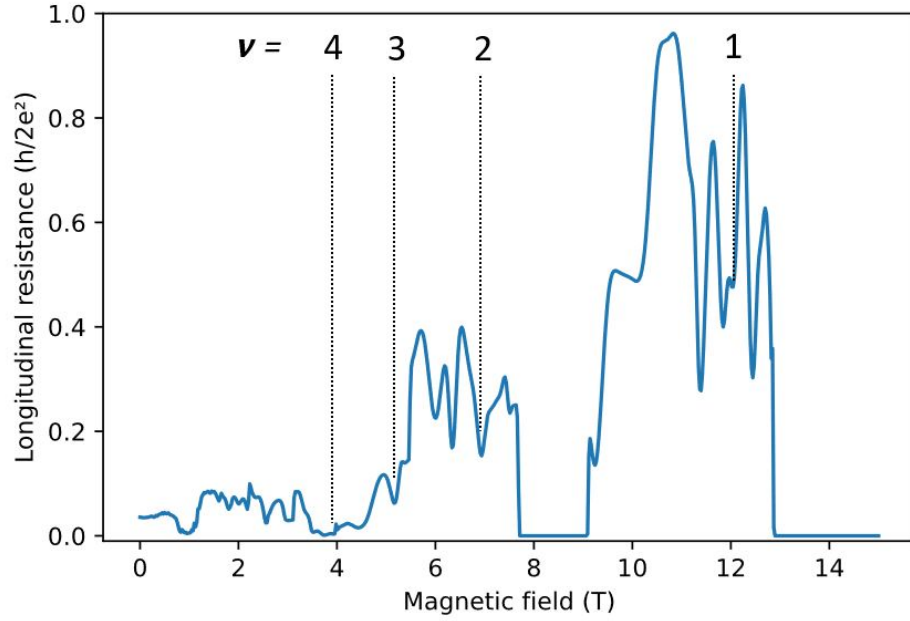


Figure 5.8: Longitudinal resistance as a function of B. One can observe the apparition of a plateau at around 10T.

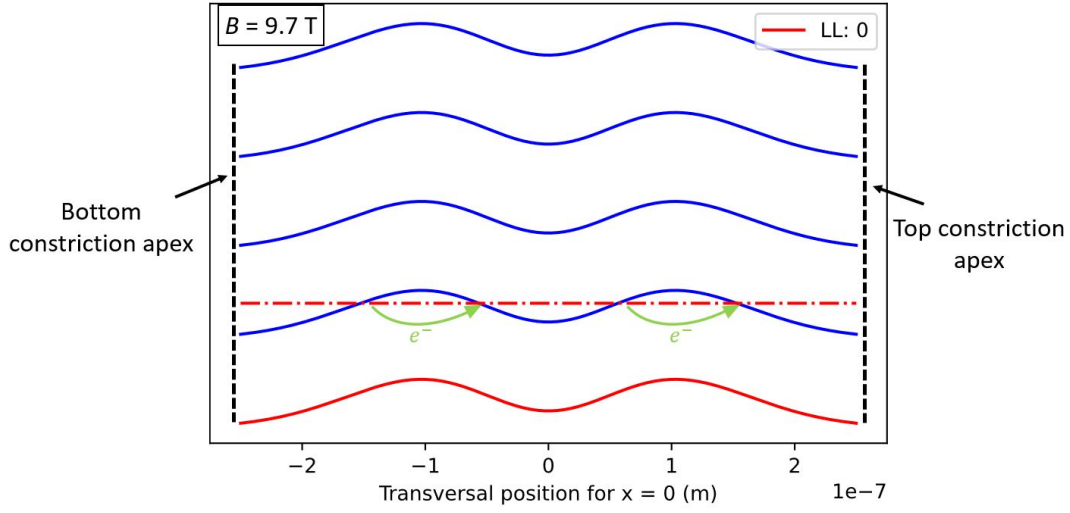


Figure 5.9: Energy bands in a transverse cross section for $x=0$. The Fermi energy is represented in a red dotted line. The black dotted lines represent the apex of the each side of the constriction. In green, the probability of tunneling of electrons to the QHI.

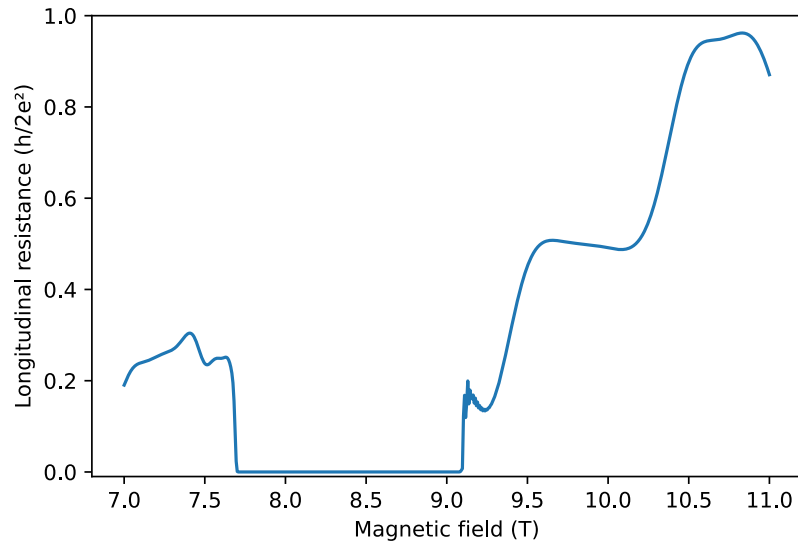


Figure 5.10: Longitudinal resistance between 7 and 11 T. It shows a plateau between 9.5 and 10 T corresponding to the coupling of the LL $n = 1$ with the QHI.

Chapter 6

Conclusion and perspectives

This master thesis had for purpose to demonstrate the ability of manipulating ESs of graphene in the QHE regime with the help of a SGM tip. Specifically, understanding the mechanisms appearing when edge channels couple with the QHI, leading to oscillations of the resistance.

The simulations gave the liberty to try different geometries or different sets of parameters without all the disadvantages of the experimental part. The simulation part of the master thesis introduced two different graphene geometries trying to highlight interferences. The first one is a device with one constriction and a tip potential at the center allowing to change the path of the edge state and to control the reflection and transmission coefficient. The second one is a device with two constrictions between which a tip potential is introduced allowing only to change the path of the edge states. In that device the reflection and transmission coefficient are controlled by the size of the constrictions.

Concerning the single constriction, the variation of the coupling between the QHI and a edge channel highlighted changes in the amplitude of resistance oscillations. Also, R_{xx} has been shown to be quite sensitive to the positioning of the SGM tip in the constriction. A slight shift from the center leads to different coupling regimes.

Concerning the double constriction, several things have been pointed out. First, the impact of the constriction aperture on the interferometer. Secondly, resistance oscillations for channels that do not interact with the tip potential. In addition, Fabry-Pérot cavity with two or more edge channels have been detailed and grasped with a simple model.

The fabrication process has been a trickier part. The first steps of exfoliation, selection and stacking have gone well by following the guidelines of the previous master thesis. Unfortunately, due to a breakdown of the e-beam lithography in the Winfab, the stacks have been sent to the University of Paris to complete the remaining steps. The first stack has been cut in half by the etching of the constriction. The second one has return with the expected single and double constriction. The bonding has been done and the device was ready to test but it turns out that no current was flowing between any leads. There had also renovations made in the laboratory used for low-temperature and high magnetic field generation. So, even formerly working graphene Hall bar could not have be tested.

A lot of improvement and perspectives are possible in the electronic interferometry field. First of all concerning the perspective as part of the achievement of the master thesis. It could be interesting to improve the transfer technique which time-consuming and still a hazardous process. Moreover, it is very difficult to stake layers if the flakes are large or near the edges of the wafer. The repetition of the pick up might also generate wrinkles in the layers; which is perhaps a reason among others explaining experimental failure of this work. Another improvement would be the attachment of a graphite back gate giving an additional degree of freedom to control the electronic band structure. Side gates could also be a great add-on to the device. Indeed, it enables a better control of the edge state in the constriction and brings modularity to experiments.

From a more comprehensive perspective, electronic interferometry in nanostructures has a bright future ahead. One of the main reason of this excitement is quantum supremacy coming around the corner. Quantum-Hall edge state interferometry is serious a candidate amongst others to achieve that. Research groups have already implemented an universal set of quantum gates for flying-quantum bits via an electronic Mach-Zehnder interferometer [4]. From another point of view, recent advances in coupling graphene QH edge channels with superconductivity [74] may lead to new kind of interferometry devices...

Acknowledgments

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First and foremost, we would like to thanks our supervisor *Pr. Benoît Hackens* for giving us the opportunity to work on this exciting topic. He made himself available in numerous times to discuss the advancement of the project as well as getting us back on track when our ideas lost us. He has been full of precious advices and made the connection with its friendly research group. Speaking of which, we would like to express our deepest gratitude to Nicolas Moreau that has by our side so many times. He demonstrates relentless devotion to help in the simulations, in the laboratory or in the general comprehension of the physics.

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We do not omit Mr. Miloud Zitout that kindly performed the bonding operation for the stack.

Finally, we would like to express our deep appreciation to our families that have been supportive through the ups and downs of the thesis.

To end on a lighter touch, a big thank you to Microsoft Teams that keep us in touch while working during this pandemic.

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Chapter 7

Supplementary information

7.1 Fabrication



Figure 7.1: Microscope capture of BN flakes for a second stack.

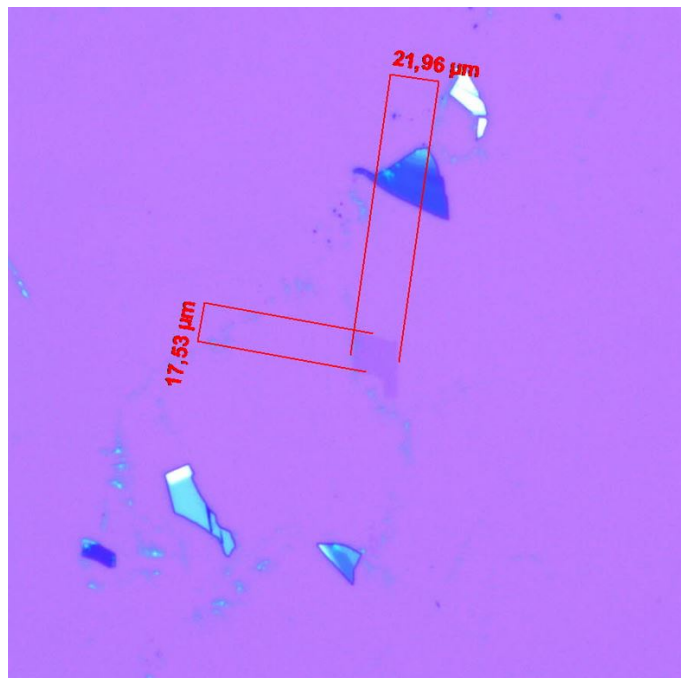


Figure 7.2: Microscope capture of graphene for a second stack.

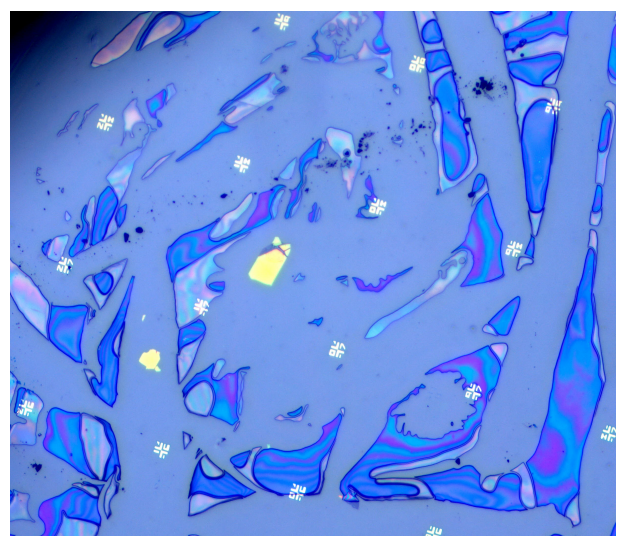
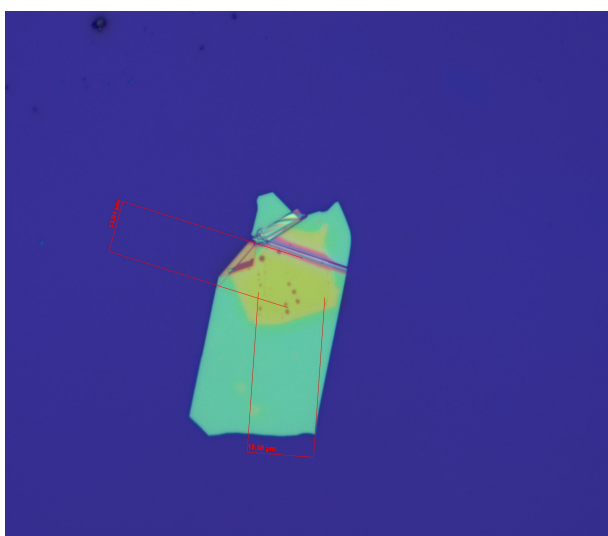


Figure 7.3: On the left: Second stack on Si/SiO_2 . On the right: On the right: Deposition of the second stack with the PPC on marked wafer.

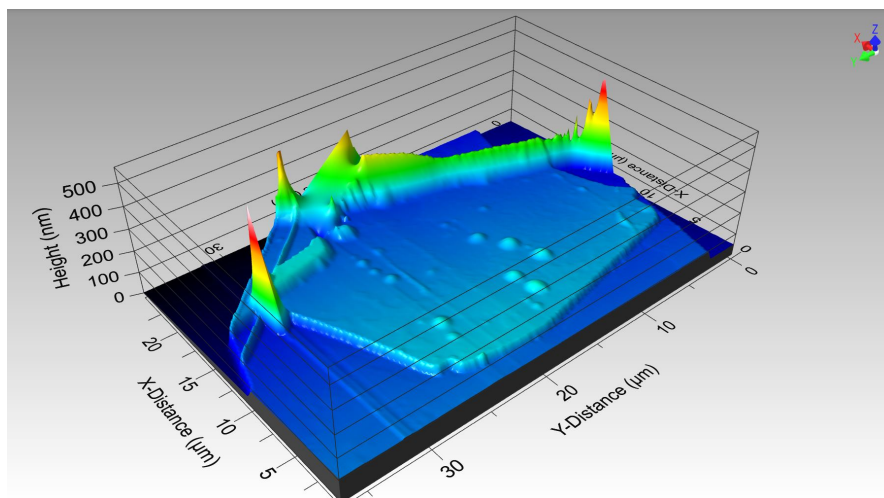


Figure 7.4: AFM capture of the 3D topology of the second stack.

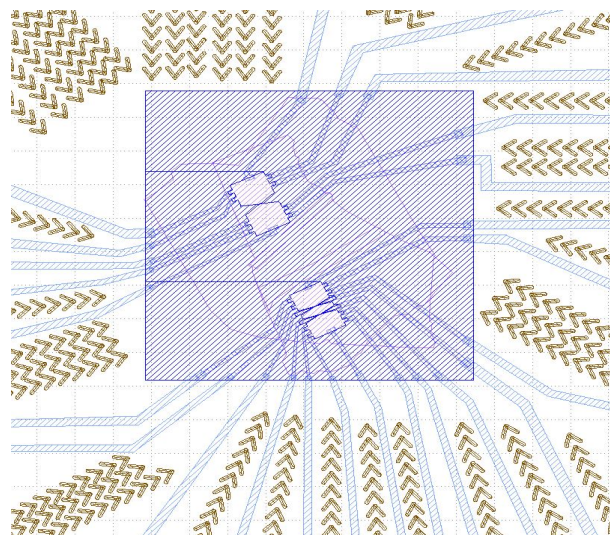
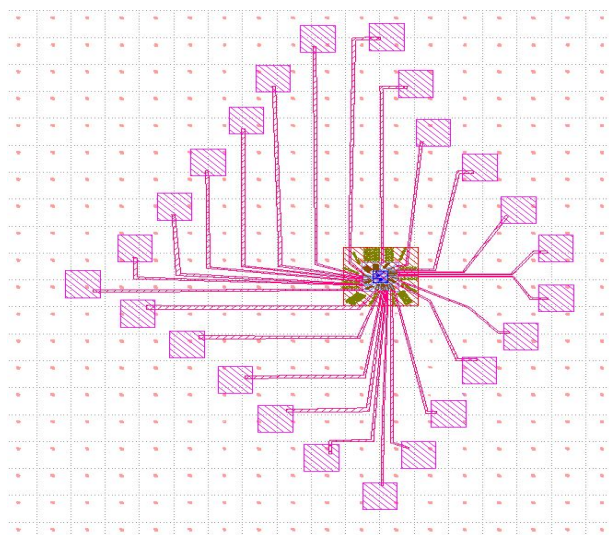


Figure 7.5: Lithography file used for the e-beam lithography of the first stack.

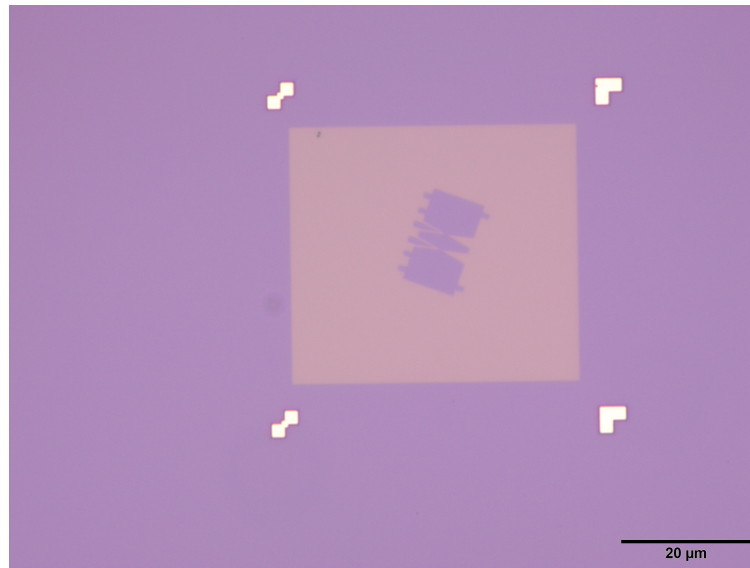


Figure 7.6: Test of dosing of the e-beam lithography.

7.2 Kwant codes

7.2.1 Single constriction code

This section introduce lines of code used to generate the results obtained for the single constriction.

```
1 import kwant
2 import scipy
3 import numpy as np
4 from matplotlib import pyplot as plt
5 from types import SimpleNamespace
6
7
8 h      = 6.626069e-34      # Planck constant (Js)
9 e      = 1.602e-19        # electron charge (C)
10 c      = 299792458        # Light celerity (m/s)
11 kB     = 1.3806503e-23    # Boltzmann constant (kg m2/Ks2)
12 m_e    = 9.1e-31         # electron mass (kg)
13 h_bar  = h/(2*np.pi)
14
15
16 asquare = 0.246e-9# [m] a is the lattice parameter
17 tsquare = 2.8 # [eV] t is the hopping parameter
18
19 scaling = 8 # scaling factor
20
21 """scaling"""
22
23 al = asquare * scaling
24 t  = tsquare / scaling
25 print("Max value Ef: {} eV".format(t*0.5))
26
27
28 #Basic system's parameters
29 W = 500e-9 ; L = 1000e-9 # width and length of the electronic system
30
31 width_leads = 10e-9 # width of the small leads of the Hall bar
32 posL        = 1000e-9/3 # pos of the leads along x
33 #posL = 4e-7
34 lead_ext    = posL + width_leads/2
35 lead_int    = posL - width_leads/2
36
37 #Indentation's parameters
38 height_indentation    = 125e-9
39 length_indentation    = 200e-9
40 position_indentation1 = (0, -W/2)
41 position_indentation2 = (0, W/2)
42
43 #Potential parameters
44 #sigma = (7.458e-8, 7.458e-8)
45 #sigma = (7.4072e-8, 7.4072e-8)
46 sigma = (7.4e-8, 7.4e-8)
47 center = (0,0)
48
49
```

```

50 #Construction of the indentation
51 def geom(pos):
52     x, y = pos
53     x_indentation1, y_indentation1 = position_indentation1 #Position of the bottom
54     x_indentation2, y_indentation2 = position_indentation2 #Posistion of the top
55     indentation
56     #Parameters of the bottom indentation
57     m1_indentation1 = 2*height_indentation/length_indentation
58     p1_indentation1 = y_indentation1 + height_indentation*(1-2*x_indentation1/
59     length_indentation)
60     m2_indentation1 = -m1_indentation1
61     p2_indentation1 = y_indentation1 + height_indentation*(1+2*x_indentation1/
62     length_indentation)
63     #Parameters of the top indentation
64     m1_indentation2 = m2_indentation1
65     p1_indentation2 = y_indentation2 + height_indentation*(-1+2*x_indentation2/
66     length_indentation)
67     m2_indentation2 = -m1_indentation2
68     p2_indentation2 = y_indentation2 - height_indentation*(1+2*x_indentation2/
69     length_indentation)
70     #Drawing of the bottom indentation
71     if x_indentation1 - length_indentation/2 < x < x_indentation1 and y_indentation1
72     < y < m1_indentation1*x + p1_indentation1:
73         return False
74     if x_indentation1 <= x < x_indentation1 + length_indentation/2 and y_indentation1
75     < y < m2_indentation1*x + p2_indentation1:
76         return False
77     #Drawing of the top indentation
78     if x_indentation2 -length_indentation/2 < x < x_indentation2 and m1_indentation2*
79     x + p1_indentation2 < y < y_indentation2:
80         return False
81     if x_indentation2 <= x < x_indentation2 + length_indentation/2 and
82     m2_indentation2*x + p2_indentation2 < y < y_indentation2:
83         return False
84     elif -L/2 < x < L/2 and -W/2 < y < W/2:
85         return True
86     else:
87         return False
88     def lead_shape(pos):
89         x, y = pos
90         return -W/2 < y < W/2
91     def lead_shape_left(pos):
92         x, y = pos
93         return -lead_ext < x < -lead_int
94     def lead_shape_right(pos):

```

```

96     x, y = pos
97     return lead_ext > x > lead_int
98
99
100 #Gaussienne shape for the tip potential
101 def gauss(site, center, sigma, amplitude):
102     x, y = site.pos
103     x0, y0 = center
104     sigmax, sigmay = sigma
105
106     return amplitude*np.exp(-((x - x0)**2)/(2*sigmax**2) - ((y - y0)**2)/(2*sigmay
107     **2))
108
109
110 def onsite(site):
111     return Vg + gauss(site, center, sigma, Vtip)
112
113
114 def disorder(site):
115     x, y = site.pos
116     pot = np.random.normal(0,0.015*t)
117
118     return pot
119
120
121 def hopping(site_i, site_j):
122     xi, yi = site_i.pos
123     xj, yj = site_j.pos
124
125     """ Change the definition of hop to include the magnetic field Bfield in the
126     definition of the hopping parameter """
127
128     hop = t*np.exp(np.pi*1j*e*Bfield*(yi+yj)*(xj-xi)/h)
129
130     return hop
131
132 def sys_builder():
133     graphene = kwant.lattice.general([(np.sqrt(3)*al, 0), (0, 3*al)], [(al*np.sqrt(3)
134     /2, 0), (0, al/2), (0, 3*al/2), (al*np.sqrt(3)/2, 2*al)], norbs = 1)
135     A, B, C, D = graphene.sublattices
136     sys = kwant.Builder()
137
138     sys[graphene.shape(geom, (0,0))] = onsite
139
140     hoppings = (((0, 0), B, A), ((0, 0), C, B), ((0, 0), D, C), ((-1, 0), A, B),
141     ((-1, 0), D, C), ((0, 1), A, D)) # the function hopping is given on each edge
142     sys[[kwant.builder.HoppingKind(*hopping) for hopping in hoppings]] = hopping
143
144
145     """ Lead 1 """
146     sym0 = kwant.TranslationalSymmetry(graphene.vec((-1, 0)))
147     lead0 = kwant.Builder(sym0)

```

```

148     lead0[graphene.shape(lead_shape, (0, 0))] = 0
149     lead0[graphene.neighbors()] = hopping
150
151     """ Lead 2 """
152     sym1 = kwant.TranslationalSymmetry(graphene.vec((1, 0)))
153     lead1 = kwant.Builder(sym1)
154     lead1[graphene.shape(lead_shape, (0, 0))] = 0
155     lead1[graphene.neighbors()] = hopping
156
157     """ Lead 5 """
158     sym4 = kwant.TranslationalSymmetry(graphene.vec((0, 1)))
159     lead4 = kwant.Builder(sym4)
160     lead4[graphene.shape(lead_shape_left, (-posL, 0))] = 0
161     lead4[graphene.neighbors()] = hopping
162
163
164
165     """ Lead 3 """
166     #sym2 = kwant.TranslationalSymmetry(graphene.vec((0, 1)))
167     lead2 = kwant.Builder(sym4)
168     lead2[graphene.shape(lead_shape_right, (posL, 0))] = 0
169     lead2[graphene.neighbors()] = hopping
170
171
172
173     """ Lead 4 """
174     sym3 = kwant.TranslationalSymmetry(graphene.vec((0, -1)))
175     lead3 = kwant.Builder(sym3)
176     lead3[graphene.shape(lead_shape_left, (-posL, 0))] = 0
177     lead3[graphene.neighbors()] = hopping
178
179
180
181
182
183     sys.attach_lead(lead0)
184     sys.attach_lead(lead1)
185     sys.attach_lead(lead2)
186     sys.attach_lead(lead3)
187     sys.attach_lead(lead4)
188
189     sys = sys.finalized()
190     return sys
191     """ Schematic of the Hall bar """
192
193
194
195 #
196 #
197 #
198 #
199 #
200 #
201 #
202 #
203 #

```

,-----o-----Vxx-----.
 # | Lead 3 | | | Lead 5 |---|---|
 # Vxy ---| |---| |---|---| (ground)
 # | | I | |
 # | Lead 1 |--->| Lead 2 |
 # | |---| |---|
 # | | | |
 # | Lead 4 | | | not implemented (because not necessary)

```
204 sys = sys_builder()
205
206
207
208 def poltsys():
209     kwant.plot(sys, site_size = 1e-9)
210
211 poltsys()
212
213
214 Ef = 0.175
215 if Ef > 0.5*t:
216     print('\033[31m' + "Warning, Ef is too high !")
217     print('\033[0m')
218     exit
219
220 #Bfield = (2*Ef**2*h_bar)/(9*t**2*al**2*e*0.5) # to be completed
221 Bfield = 8
222
223 """ Parameter for the zero density zone """
224 Vg      = 0
225 Vtip    = 0.0
226 params  = dict(Bfield=Bfield, Vg = Vg) # params take the magnetic field as a
227     parameter for the function hopping
228
229 """ The wavelength must be (much more) larger than the lattice parameter """
230 lambda_F = 2 * np.pi * al * np.sqrt(t / Ef) # computation of the wavelength
231 if lambda_F/al < 2:
232     print('Warning : lambda_F must be larger than the lattice parameter a')
233
234
235 num_LL = 5
236
237 plt.figure()
238
239 for n in range(num_LL):
240
241     """
242     Change the definition of En to calculate the Landau levels energy as a function
243     of
244     the magnetic field Bfield and the Landau level label n
245
246     """
247     vf      = (3*t*al)/(2*h_bar)
248     Enp     = vf*np.sqrt(2*h_bar*e)*np.sqrt(n*Bfield) # to be completed
249     Enm     = -Enp
250
251     x = np.array([0, 1]) ; y = Enp*np.array([1, 1]) ; z = Enm*np.array([1, 1]) # in
252     order to plot the Landau levels
253     plt.plot(x, y, 'b')
254     plt.plot(x, z, 'b')
255
256 plt.plot(x, Ef*np.array([1, 1]), 'r-') # to plot the Fermi energy (in red)
257
258 plt.xlabel('DOS (a.u.)')
```

```

257 plt.ylabel('Energy (eV)')
258
259 plt.show()
260
261
262 Vtip = 0.05
263 vals=[onsite(sys.sites[n]) for n in range(sys.graph.num_nodes)]
264 kwant.plotter.map(sys, vals, cmap = 'RdBu', vmin=0, vmax = Vtip)
265
266
267 #para = np.linspace(7.2e-8,7.25e-8,10)
268 para = [7.055e-8]
269 Ef = 0.175
270 Vtip = 0.05
271 for i, w in enumerate(para):
272     #center = (0, w)
273     sigma = (w,w)
274     #sys = sys_builder()
275     wfs = kwant.wave_function(sys, energy=Ef, params = params) # the wave function is
276                                     # parameters in
277     arguments
278     scattering_wf = wfs(0) # all scattering wave functions from lead 0
279     J0 = kwant.operator.Current(sys)
280     wf_left = wfs(0)
281
282     current = sum(J0(p, params = params) for p in wf_left) # to sum over all the lead
283     's mode
284
285     kwant.plotter.current(sys, current, cmap='viridis')
286
287
288 #Simul
289 #Variation of the magnetic field
290 import time
291
292 Ef = 0.175
293 V_tip = [0.05]
294 length_indentation = 200e-9 #Initial indentation length
295 height_indentation = 125e-9
296 Bfields = np.linspace(7.5,8.25, 200)
297 Rxys = np.zeros([len(V_tip),len(Bfields)])
298 Rxys = np.zeros([len(V_tip),len(Bfields)])
299 sys = sys_builder()
300 #Gxys = np.zeros([len(Bs),1])
301 #Gxys = np.zeros([len(Bs),1])
302
303 """
304 The code below is used to compute the Hall and the longitudinal resistivity. It is
305 based on a solution proposed by
306 Anton Akhmerov on the Kwant forum at the adress https://www.mail-archive.com/kwant-discuss@kwant-project.org/msg00110.html
307 """
308
309 for j, tip in enumerate(V_tip):
310     print("Tip: {}".format(tip))

```

```

308
309     for i, s in enumerate(Bfields):
310         try:
311             if i == 0:
312                 myTime = time.time()
313                 print(s)
314                 Vtip = tip
315                 Bfield = s
316                 params = dict(Bfield=Bfield, Vg = 0)
317                 s = kwant.smatrix(sys, energy = Ef, params = params) #
transmission matrix (here this)
318
319             # First we calculate the conductance matrix given the scattering matrix S
320             cond = np.array([[s.transmission(i, j) for j in range(n)] for i in range(
n)])
321
322             # Correct the reflection blocks, so that rows and columns sum to zero.
323             cond -= np.diag(cond.sum(axis=0)) # a -= b means a = a-b
324
325             # In order to calculate the nonlocal conductance we eliminate one row and
one column
326             # from the conductance matrix. This amounts to setting the corresponding
voltage to zero
327             # and using current conservation to calculate the current through the
last terminal.
328             # This is equivalent to put V_5 (lead 5) to the ground (V_5 = 0)
329             cm = s.conductance_matrix()[:-1, :-1] #Permet de mettre un contacte à la
masse, retir une ligne et une colonne
330
331             # We then set the current to be 1 in the lead 0, -1 in lead 2, and
332             # calculate the voltage in lead 1 (so V_3 - V_5 since V_5 = 0).
333             Rxx = np.linalg.solve(cm, [1, -1, 0, 0])[2] #indice entre crochet ce sont
les courant 1 = injecte un courant, -1 = courant qui arrive donc d'
office 1 et -1. Indice 2, indice de la résistance Indice 2 = V3
334
335             Rxxs[j][i] = Rxx
336
337             # The same for V_4-V_5 (Hall resistance)
338             Rxy = np.linalg.solve(cm, [1, -1, 0, 0])[3] # to be completed
339             Rxys[j][i] = Rxy
340             #Gxx = 1/Rxx
341             #Gxxs[i] = Gxx
342             print('iteration', i, 'succeeded')
343             print('Resistance value', Rxx)
344         except Exception as ex:
345             print('problem encountered at iteration', i)
346             print('Warning :', ex)
347
348     finally:
349         if i == 0:
350             remainingTime = (time.time() - myTime)*len(Bfields)*(len(V_tip)-j)
351             print('Remaining time :')
352             print(time.strftime("%H:%M:%S", time.gmtime(remainingTime)))
353
354
355 plt.figure()

```

```

356 for index, valeurtip in enumerate(V_tip):
357     #plt.plot(Distance, Rxys[index], label = 'Rxy Vtip: {}'.format(valeurtip))
358     plt.plot(Bfields, -Rxxs[index], label = 'Rxx Vtip: {}'.format(valeurtip))
359
360 plt.legend()
361
362 plt.xlabel('Magnetic field (T)')
363
364 plt.ylabel('Longitudinal resistance ( $h/2e^2$ )')
365 plt.savefig('RxxSample1Field.svg', bbox_inches='tight', dpi = 1200)
366 #plt.figtext(.72, .8, "B = 8T")
367 #plt.figtext(.72, .75, "Scaling = 8")
368 plt.show()
369
370
371 #Simu2
372 #Variation of the potential width
373 import time
374
375 Ef = 0.175
376 V_tip = [0.05]
377 length_indentation = 200e-9 #Initial indentation length
378 height_indentation = 125e-9
379 widthPot = np.linspace(0.7e-7, 0.85e-7, 1000)
380 Rxxs = np.zeros([len(V_tip), len(widthPot)])
381 Rxys = np.zeros([len(V_tip), len(widthPot)])
382
383 sys = sys_builder()
384 #Gxys = np.zeros([len(Bs), 1])
385 #Gxxs = np.zeros([len(Bs), 1])
386
387 """
388 The code below is used to compute the Hall and the longitudinal resistivity. It is
389 based on a solution proposed by
390 Anton Akhmerov on the Kwant forum at the adress https://www.mail-archive.com/kwant-discuss@kwant-project.org/msg00110.html
391 """
392 for j, tip in enumerate(V_tip):
393     print("Tip: {}".format(tip))
394     for i, s in enumerate(widthPot):
395         try:
396             if i == 0:
397                 myTime = time.time()
398                 print(s)
399                 Vtip = tip
400                 sigma = (s, s)
401                 params = dict(Bfield=Bfield, Vg = 0)
402                 s = kwant.smatrix(sys, energy = Ef, params = params) #
403                 transmission matrix (here this)
404
405                 # First we calculate the conductance matrix given the scattering matrix S
406                 cond = np.array([[s.transmission(i, j) for j in range(n)] for i in range(
407                     n)])

```

```

408     # Correct the reflection blocks, so that rows and columns sum to zero.
409     cond == np.diag(cond.sum(axis=0)) # a == b means a = a-b
410
411     # In order to calculate the nonlocal conductance we eliminate one row and
412     # one column
413     # from the conductance matrix. This amounts to setting the corresponding
414     # voltage to zero
415     # and using current conservation to calculate the current through the
416     # last terminal.
417     # This is equivalent to put V_5 (lead 5) to the ground (V_5 = 0)
418     cm = s.conductance_matrix()[:-1, :-1] #Permet de mettre un contacte à la
419     # masse, retir une ligne et une colonne
420
421     # We then set the current to be 1 in the lead 0, -1 in lead 2, and
422     # calculate the voltage in lead 1 (so V_3 - V_5 since V_5 = 0).
423     Rxx = np.linalg.solve(cm, [1, -1, 0, 0])[2] #indice entre crochet ce sont
424     # les courant 1 = injecte un courant, -1 = courant qui arrive donc d'
425     # office 1 et -1. Indice 2, indice de la résistance Indice 2 = V3
426
427     Rxys[j][i] = Rxx
428
429     # The same for V_4-V_5 (Hall resistance)
430     Rxy = np.linalg.solve(cm, [1, -1, 0, 0])[3] # to be completed
431     Rxys[j][i] = Rxy
432     #Gxx = 1/Rxx
433     #Gxxs[i] = Gxx
434     print('iteration', i, 'succeeded')
435     print('Resistance value', Rxx)
436 except Exception as ex:
437     print('problem encountered at iteration', i)
438     print('Warning :', ex)
439
440 finally:
441     if i == 0:
442         remainingTime = (time.time() - myTime)*len(widthPot)*(len(V_tip)-j)
443         print('Remaining time :')
444         print(time.strftime("%H:%M:%S", time.gmtime(remainingTime)))
445
446 plt.figure()
447
448 for index, valeurtip in enumerate(V_tip):
449     #plt.plot(Distance, Rxys[index], label = 'Rxy Vtip: {}'.format(valeurtip))
450     plt.plot(widthPot, -Rxys[index], label = 'Rxx Vtip: {}'.format(valeurtip))
451
452 plt.legend()
453
454 plt.xlabel('Potential width (m)')
455
456 plt.ylabel('Longitudinal resistance (h/2e^2)')
457 #plt.savefig('RxxSample1V005ENSEMBLELEAD2.svg',bbox_inches='tight', dpi = 1200)
458 #plt.figtext(.72, .8, "B = 8T")
459 #plt.figtext(.72, .75, "Scaling = 8")
460 plt.show()

```

```

458 #Simu3
459 #Variation of the indentation height
460 import time
461
462 Ef = 0.1
463 Vtip = 0
464 length_indentation = 200e-9 #Initial indentation length
465 height_indentations = np.linspace(230e-9, 236e-9, 300)
466 widthPot = [0.1]
467 Rxxs = np.zeros([len(widthPot), len(height_indentations)])
468 Rxys = np.zeros([len(widthPot), len(height_indentations)])
469 Bfield = 8
470 #Gxys = np.zeros([len(Bs), 1])
471 #Gxxs = np.zeros([len(Bs), 1])
472
473 """
474 The code below is used to compute the Hall and the longitudinal resistivity. It is
475 based on a solution proposed by
476 Anton Akhmerov on the Kwant forum at the adress https://www.mail-archive.com/kwant-discuss@kwant-project.org/msg00110.html
477 """
478 for j, tip in enumerate(widthPot):
479     print("Tip width: {}".format(tip))
480     sigma = (tip, tip)
481     for i, p in enumerate(height_indentations):
482         try:
483             if i == 0:
484                 myTime = time.time()
485                 print("Height: {}".format(p))
486                 height_indentation = p
487                 params = dict(Bfield=Bfield, Vg = 0)
488                 sys = sys_builder()
489                 s = kwant.smatrix(sys, energy = Ef, params = params) #
490                 transmission matrix (here this)
491
492                 # First we calculate the conductance matrix given the scattering matrix S
493                 cond = np.array([[s.transmission(i, j) for j in range(n)] for i in range(
494                     n)])
495
496                 # Correct the reflection blocks, so that rows and columns sum to zero.
497                 cond -= np.diag(cond.sum(axis=0)) # a -= b means a = a-b
498
499                 # In order to calculate the nonlocal conductance we eliminate one row and
500                 one column
501                 # from the conductance matrix. This amounts to setting the corresponding
502                 voltage to zero
503                 # and using current conservation to calculate the current through the
504                 last terminal.
505                 # This is equivalent to put V_5 (lead 5) to the ground (V_5 = 0)
506                 cm = s.conductance_matrix()[:-1, :-1] #Permet de mettre un contacte à la
507                 masse, retir une ligne et une colonne
508
509                 # We then set the current to be 1 in the lead 0, -1 in lead 2, and
510                 # calculate the voltage in lead 1 (so V_3 - V_5 since V_5 = 0).
511                 Rxx = np.linalg.solve(cm, [1, -1, 0, 0])[2] #indice entre crochet ce sont

```

```

les courant 1 = injecte un courant, -1 = courant qui arrive donc d'
office 1 et -1. Indice 2, indice de la résistance Indice 2 = V3
506
507     if Rxx < -3:
508         Rxx = -3
509     Rxxs[j][i] = Rxx
510
511     # The same for V_4-V_5 (Hall resistance)
512     Rxy = np.linalg.solve(cm, [1, -1, 0, 0])[3] # to be completed
513     Rxys[j][i] = Rxy
514
515     if Rxx < -4:
516         Rxx = -4
517
518     #Gxx = 1/Rxx
519     #Gxxs[i] = Gxx
520     print('iteration', i, 'succeeded')
521     print('Resistance value', Rxx)
522 except Exception as ex:
523     print('problem encountered at iteration', i)
524     print('Warning:', ex)
525
526 finally:
527     if i == 0:
528         remainingTime = (time.time() - myTime)*len(height_indentations)*(len(
widthPot)-j)
529         print('Remaining time:')
530         print(time.strftime("%H:%M:%S", time.gmtime(remainingTime)))
531
532
533 plt.figure()
534
535 for index, largeurTip in enumerate(widthPot):
536     #plt.plot(Distance, Rxys[index], label = 'Rxy Vtip: {}'.format(valeurtip))
537     plt.plot(height_indentations, -Rxxs[index])
538
539
540 plt.xlabel('Indentation depth (m)')
541 plt.ylabel('Longitudinal resistance ( $h/2e^2$ )')
542 plt.savefig('zoomIndentationDepthSample1.svg', bbox_inches='tight', dpi = 1200)
543 #plt.figtext(.70, .63, "B = 1T")
544 #plt.figtext(.70, .58, "Scaling = 20")
545 plt.show()
546
547
548 plt.figure()
549
550 for index, positionTip in enumerate(positions):
551     #plt.plot(Distance, Rxys[index], label = 'Rxy Vtip: {}'.format(valeurtip))
552     plt.plot(widthPots, -Rxxs[index], label = 'Tip position: ({}, 0)'.format(
positionTip))
553
554 plt.legend()
555
556 plt.xlabel('Potential width (m)')
557 plt.ylabel('Longitudinal resistance ( $h/2e^2$ )')

```

```

558 plt.savefig('RxxSample1PositionHori.svg',bbox_inches='tight', dpi = 1200)
559 #plt.figtext(.70, .63, "B = 1T")
560 #plt.figtext(.70, .58, "Scaling = 20")
561 plt.show()
562
563
564 #Energy Bands
565 def energy_space_longitudinal(Fermi):
566     space = np.linspace(-L/2, L/2, 100000)
567     Enp = np.zeros(len(space))
568     Enm = np.zeros(len(space))
569     plt.figure()
570
571     for n in range(num_LL):
572         for i in range(len(space)):
573             site = kwant.builder.Site
574             site.pos = (space[i], 0)
575             vf = (3*t*al)/(2*h_bar)
576             Enp[i] = vf*np.sqrt(2*h_bar*e)*np.sqrt(n*Bfield) + onsite(site)#
to be completed
577             Enm[i] = -vf*np.sqrt(2*h_bar*e)*np.sqrt(n*Bfield) + onsite(site)
578
579             if Enp[i] > Fermi - 0.000001*Fermi and Enp[i]<Fermi +0.000001*Fermi:
580                 print("rayon : ", space[i])
581                 print("surface : ", np.pi*space[i]**2)
582
583             if n == 0:
584                 plt.plot(space,Enp,'r', label = 'LL: 0')
585                 plt.legend()
586
587             else:
588                 plt.plot(space,Enp,'b')
589                 plt.plot(space,Enm,'b')
590
591     plt.plot(space, Ef*np.array([1 for i in range(len(space))]), 'r-')
592     plt.ticklabel_format(style='sci', axis='x', scilimits=(0,0))
593     plt.xlabel('Longitudinal position for y = 0 (m)')
594     plt.ylabel('Energy (eV)')
595     #plt.savefig('Longitudinal-L400e-9-H0,75e-7-Ef0,07-V0,05-sigma2e-7.svg',
bbox_inches='tight', dpi = 1200)
596     plt.show()
597
598 Ef = 0.1
599 Vtip = 0.0
600 energy_space_longitudinal(Ef)
601
602
603 def energy_space_transversal():
604     space = np.linspace(-W/2, W/2, 100)
605     Enp = np.zeros(len(space))
606     Enm = np.zeros(len(space))
607     plt.figure()
608
609     for n in range(num_LL):
610         for i in range(len(space)):
611             site = kwant.builder.Site

```

```

612         site.pos      = (0, space[i])
613         vf             = (3*t*al)/(2*h_bar)
614         Enp[i]         = vf*np.sqrt(2*h_bar*e)*np.sqrt(n*Bfield) + onsite(site) # to
be completed
615         Emn[i]         = -vf*np.sqrt(2*h_bar*e)*np.sqrt(n*Bfield) + onsite(site)
616         if n == 0:
617             plt.plot(space, Enp, 'r', label = 'LL: 0')
618             plt.legend()
619
620         else:
621             plt.plot(space, Enp, 'b')
622             plt.plot(space, Emn, 'b')
623
624         plt.plot(space, Ef*np.array([1 for i in range(len(space))]), 'r-')
625         plt.ticklabel_format(style='sci', axis='x', scilimits=(0,0))
626         plt.xlabel('Transversal position for x = 0 (m)')
627         plt.ylabel('Energy (eV)')
628         #plt.savefig('transversal-L400e-9-H0,75e-7-Ef0,07-V0,05-sigma2e-7.svg',
bbox_inches='tight', dpi = 1200)
629         plt.show()
630
631 energy_space_transversal()

```

7.2.2 Double constriction code

This section introduce lines of code used to generate the results obtained for the double constriction.

```

1  import kwant
2  import scipy
3  import numpy as np
4  from matplotlib import pyplot as plt
5  from types import SimpleNamespace
6
7
8  h      = 6.626069e-34    # Planck constant (Js)
9  e      = 1.602e-19      # electron charge (C)
10 c      = 299792458      # Light celerity (m/s)
11 kB     = 1.3806503e-23  # Boltzmann constant (kg m2/Ks2)
12 m_e    = 9.1e-31        # electron mass (kg)
13 h_bar  = h/(2*np.pi)
14
15
16 asquare = 0.246e-9 # [m] a is the lattice parameter
17 tsquare = 2.8 # [eV] t is the hopping parameter
18
19 scaling = 8 # scaling factor
20
21 """scaling"""
22
23 al = asquare * scaling
24 t  = tsquare / scaling
25 print("Max value Ef: {} eV".format(t*0.5))
26

```

```

27
28 #Basic system's parameters
29 W = 500e-9 ; L = 1000e-9 # width and length of the electronic system
30 width_leads = 5e-9 # width of the small leads of the Hall bar
31 posL = 400e-9 # pos of the leads along x
32 lead_ext = posL + width_leads/2
33 lead_int = posL - width_leads/2
34
35 #Indentation 1 is the bottom one and 2 the upper one
36
37 # Right indentations parameters
38 height_indentation = 235e-9 #hauteur des indentations
39 length_indentation = 200e-9 #Largeur indentations
40 position_indentation1_right = (L/4, -W/2)
41 position_indentation2_right = (L/4, W/2)
42
43 #Right indentations parameters
44 position_indentation1_left = (-L/4, -W/2)
45 position_indentation2_left = (-L/4, W/2)
46
47 #Tip parameter Gaussienne
48 Vtip = 0.05
49 sigmaTip = (0.25e-7, 0.25e-7)
50 centerTip = (0, -W/2)
51
52
53 #Tip parameter rectangle
54 hauteurRectangle = 0.75e-7
55 largeurRectangle = 1e-7
56
57
58 def indentation(pos, position1, position2, height, length):
59     x,y = pos
60     x_indentation1, y_indentation1 = position1 #Position of the bottom indentation
61     x_indentation2, y_indentation2 = position2 #Position of the top indentation
62
63     #Parameters of the bottom indentation
64     m1_indentation1 = 2*height/length
65     p1_indentation1 = y_indentation1 + height*(1-2*x_indentation1/length)
66     m2_indentation1 = -m1_indentation1
67     p2_indentation1 = y_indentation1 + height*(1+2*x_indentation1/length)
68
69     #Parameters of the top indentation
70     m1_indentation2 = m2_indentation1
71     p1_indentation2 = y_indentation2 + height*(-1+2*x_indentation2/length)
72     m2_indentation2 = -m1_indentation2
73     p2_indentation2 = y_indentation2 - height*(1+2*x_indentation2/length)
74
75     #Drawing of the bottom indentation
76     if x_indentation1 - length/2 < x < x_indentation1 and y_indentation1 < y <
m1_indentation1*x + p1_indentation1:
77         return False
78     if x_indentation1 <= x < x_indentation1 + length/2 and y_indentation1 < y <
m2_indentation1*x + p2_indentation1:
79         return False
80

```

```
81 #Drawing of the top indentation
82 if x_indentation2 - length/2 < x < x_indentation2 and m1_indentation2*x +
p1_indentation2 < y < y_indentation2:
83     return False
84 if x_indentation2 <= x < x_indentation2 + length/2 and m2_indentation2*x +
p2_indentation2 < y < y_indentation2:
85     return False
86
87 elif -L/2 < x < L/2 and -W/2 < y < W/2:
88     return True
89 else:
90     return False
91
92
93 def geom(pos):
94
95     if indentation(pos, position_indentation1_left, position_indentation2_left,
height_indentation, length_indentation) == False:
96         return False
97     elif indentation(pos, position_indentation1_right, position_indentation2_right,
height_indentation, length_indentation) == False:
98         return False
99     else:
100         return True
101
102
103 def lead_shape(pos):
104     x, y = pos
105     return -W/2 < y < W/2
106
107 def lead_shape_left(pos):
108     x, y = pos
109     return -lead_ext < x < -lead_int
110
111 def lead_shape_right(pos):
112     x, y = pos
113     return lead_ext > x > lead_int
114
115
116 def gauss(site, center, sigma, amplitude):
117     x, y = site.pos
118     x0, y0 = center
119     sigmax, sigmay = sigma
120
121     return amplitude*np.exp(-((x - x0)**2)/(2*sigmax**2) - ((y - y0)**2)/(2*sigmay
**2))
122
123
124 def rectangle(site, hauteur, largeur, amplitude):
125     x, y = site.pos
126     x0 = 0
127     y0 = -W/2
128     if x < x0 + largeur/2 and x > x0 - largeur/2:
129         if y >= y0 and y < y0 + hauteur:
130             return amplitude
131         else:
```

```

132         return 0
133     else:
134         return 0
135
136
137 def onsite(site):
138     return Vg + gauss(site, centerTip, sigmaTip, Vtip)
139     #return Vg + rectangle(site, hauteurRectangle, largeurRectangle, Vtip)
140
141
142 def hopping(site_i, site_j):
143     xi, yi = site_i.pos
144     xj, yj = site_j.pos
145
146     hop = t*np.exp(np.pi*1j*e*Bfield*(yi+yj)*(xj-xi)/h)
147
148     return hop
149
150
151 def sys_builder():
152     graphene = kwant.lattice.general([(np.sqrt(3)*al, 0), (0, 3*al)], [(al*np.sqrt(3)
153 /2, 0), (0, al/2), (0, 3*al/2), (al*np.sqrt(3)/2, 2*al)], norbs = 1)
154     A, B, C, D = graphene.sublattices
155     sys = kwant.Builder()
156
157     sys[graphene.shape(geom, (0,0))] = onsite
158
159     hoppings = (((0, 0), B, A), ((0, 0), C, B), ((0, 0), D, C), ((-1, 0), A, B),
160 ((-1, 0), D, C), ((0, 1), A, D)) # the function hopping is given on each edge
161     sys[[kwant.builder.HoppingKind(*hopping) for hopping in hoppings]] = hopping
162
163     """ Lead 1 """
164     sym0 = kwant.TranslationalSymmetry(graphene.vec((-1, 0)))
165     lead0 = kwant.Builder(sym0)
166     lead0[graphene.shape(lead_shape, (0, 0))] = 0
167     lead0[graphene.neighbors()] = hopping
168
169     """ Lead 2 """
170     sym1 = kwant.TranslationalSymmetry(graphene.vec((1, 0)))
171     lead1 = kwant.Builder(sym1)
172     lead1[graphene.shape(lead_shape, (0, 0))] = 0
173     lead1[graphene.neighbors()] = hopping
174
175     """ Lead 5 """
176     sym4 = kwant.TranslationalSymmetry(graphene.vec((0, 1)))
177     lead4 = kwant.Builder(sym4)
178     lead4[graphene.shape(lead_shape_left, (-posL, 0))] = 0
179     lead4[graphene.neighbors()] = hopping
180
181     """ Lead 3 """
182     #sym2 = kwant.TranslationalSymmetry(graphene.vec((0, 1)))
183     lead2 = kwant.Builder(sym4)
184     lead2[graphene.shape(lead_shape_right, (posL, 0))] = 0
185     lead2[graphene.neighbors()] = hopping
186
187     """ Lead 4 """

```

```

186 sym3 = kwant.TranslationalSymmetry(graphene.vec((0, -1)))
187 lead3 = kwant.Builder(sym3)
188 lead3[graphene.shape(lead_shape_left, (-posL, 0))] = 0
189 lead3[graphene.neighbors()] = hopping
190
191 sys.attach_lead(lead0)
192 sys.attach_lead(lead1)
193 sys.attach_lead(lead2)
194 sys.attach_lead(lead3)
195 sys.attach_lead(lead4)
196
197 sys = sys.finalized()
198 return sys
199
200 #### Schematic of the Hall bar ####
201 # ,-----o-----Vxx-----.
202 # | Lead 3 | | | Lead 5 |---|---'','' (ground)
203 # Vxy ---| | | |---
204 # | I
205 # | Lead 1 -----> Lead 2
206 # |---|---|---
207 # | | |
208 # | Lead 4 | not implemented (because not necessary)
209 # '-----',
210
211
212 sys = sys_builder()
213
214
215 def poltsys():
216     kwant.plot(sys, site_size = 1e-9)
217
218 poltsys()
219
220
221 Ef = 0.175
222 if Ef > 0.5*t:
223     print('\033[31m' + "Warning, Ef is too high !")
224     print('\033[0m')
225     exit
226
227 #Bfield = (2*Ef**2*h_bar)/(9*t**2*al**2*e*0.5) # to be completed
228 Bfield = 8
229
230 """ Parameter for the zero density zone """
231 Vg = 0
232 params = dict(Bfield=Bfield, Vg = Vg) # params take the magnetic field as a
    parameter for the function hopping
233
234
235 """ The wavelength must be (much more) larger than the lattice parameter """
236 lambda_F = 2 * np.pi * al * np.sqrt(t / Ef) # computation of the wavelength
237 if lambda_F/al < 2:
238     print('Warning : lambda_F must be larger than the lattice parameter a')
239
240

```

```

241 num_LL = 5
242
243 plt.figure()
244
245 for n in range(num_LL):
246
247     """
248     Change the definition of En to calculate the Landau levels energy as a function
249     of
250     the magnetic field Bfield and the Landau level label n
251
252     """
253     vf      = (3*t*al)/(2*h_bar)
254     Enp     = vf*np.sqrt(2*h_bar*e)*np.sqrt(n*Bfield) # to be completed
255     Enm     = -Enp
256
257     x = np.array([0, 1]) ; y = Enp*np.array([1, 1]) ; z = Enm*np.array([1, 1]) # in
258     order to plot the Landau levels
259     plt.plot(x, y, 'b')
260     plt.plot(x, z, 'b')
261
262 plt.plot(x, Ef*np.array([1, 1]), 'r-') # to plot the Fermi energy (in red)
263
264 plt.xlabel('DOS (a.u.)')
265 plt.ylabel('Energy (eV)')
266
267 plt.show()
268
269 vals=[onsite(sys.sites[n]) for n in range(sys.graph.num_nodes)]
270 kwant.plotter.map(sys, vals, cmap = 'RdBu', vmin=0, vmax = Vtip)
271
272 #para = [2.83e-8, 2.93e-8, 3.04e-8, 4.31e-8]
273 #para = [2.675e-8, 3.66e-8, 4.38e-8, 5.97e-8]
274 para = [2.35e-8]
275 #para = [7e-8]
276 Ef = 0.175
277 Vtip = 0.05
278 for i, w in enumerate(para):
279     sigmaTip = (w,w)
280     #hauteurRectangle = w
281     #largeurRectangle = 2e-7
282     wfs = kwant.wave_function(sys, energy=Ef, params = params) # the wave function is
283     obtained by giving the # parameters in
284     arguments
285     scattering_wf = wfs(0) # all scattering wave functions from lead 0
286     J0 = kwant.operator.Current(sys)
287     wf_left = wfs(0)
288
289     current = sum(J0(p, params = params) for p in wf_left) # to sum over all the lead
290     's mode
291
292     kwant.plotter.current(sys, current, cmap='viridis')

```

```

292
293 #Simul
294 #Variation of indentation depth
295 import time
296
297 Ef = 0.15
298 V_tip = [0.2]
299 length_indentation = 200e-9
300 height_indentations = np.linspace(230e-9, 249e-9, 300)
301 Rxxs = np.zeros([len(V_tip), len(height_indentations)])
302 Rxys = np.zeros([len(V_tip), len(height_indentations)])
303 numSyst = 1
304
305 #Gxys = np.zeros([len(Bs), 1])
306 #Gxxs = np.zeros([len(Bs), 1])
307
308 """
309 The code below is used to compute the Hall and the longitudinal resistivity. It is
    based on a solution proposed by
310 Anton Akhmerov on the Kwant forum at the address https://www.mail-archive.com/kwant-discuss@kwant-project.org/msg00110.html
311 """
312 for j, tip in enumerate(V_tip):
313
314     print("Tip: {}".format(tip))
315
316     for i, k in enumerate(height_indentations):
317         try:
318             if i == 0:
319                 myTime = time.time()
320                 Vtip = tip
321                 height_indentation = k
322                 print("Height : {}".format(k))
323                 sys = sys_builder()
324                 params = dict(Bfield=Bfield, Vg = 0)
325                 s = kwant.smatrix(sys, energy = Ef, params = params) #
    transmission matrix (here this)
326
327                 # First we calculate the conductance matrix given the scattering matrix S
328                 cond = np.array([[s.transmission(i, j) for j in range(n)] for i in range(
    n)])
329
330                 # Correct the reflection blocks, so that rows and columns sum to zero.
331                 cond -= np.diag(cond.sum(axis=0)) # a -= b means a = a-b
332
333                 # In order to calculate the nonlocal conductance we eliminate one row and
    one column
334                 # from the conductance matrix. This amounts to setting the corresponding
    voltage to zero
335                 # and using current conservation to calculate the current through the
    last terminal.
336                 # This is equivalent to put V_5 (lead 5) to the ground (V_5 = 0)
337                 cm = s.conductance_matrix()[:-1, :-1] #Permet de mettre un contacte à la
    masse, retir une ligne et une colonne
338
339                 # We then set the current to be 1 in the lead 0, -1 in lead 2, and

```

```

340         # calculate the voltage in lead 1 (so V_3 - V_5 since V_5 = 0).
341         Rxx = np.linalg.solve(cm, [1, -1, 0, 0])[2] #indice entre crochet ce sont
    les courant 1 = injecte un courant, -1 = courant qui arrive donc d'
    office 1 et -1. Indice 2, indice de la résistance Indice 2 = V3
342         if Rxx < -4:
343             Rxx = -4
344
345         Rxxs[j][i] = Rxx
346
347         # The same for V_4-V_5 (Hall resistance)
348         Rxy = np.linalg.solve(cm, [1, -1, 0, 0])[3] # to be completed
349         Rxys[j][i] = Rxy
350
351         #Gxx = 1/Rxx
352         #Gxxs[i] = Gxx
353         print('iteration', i, 'succeeded')
354         print('Resistance value', Rxx)
355     except Exception as ex:
356         print('problem encountered at iteration', i)
357         print('Warning:', ex)
358
359     finally:
360         numSyst += 1
361         if i == 0:
362             remainingTime = (time.time() - myTime)*len(height_indentations)*(len(
V_tip)-j)
363             print('Remaining time:')
364             print(time.strftime("%H:%M:%S", time.gmtime(remainingTime)))
365
366
367     plt.figure()
368
369     for index, valeurtip in enumerate(V_tip):
370         #plt.plot(Distance, Rxys[index], label = 'Rxy Vtip: {}'.format(valeurtip))
371         plt.plot(height_indentations, -Rxxs[index])
372
373
374
375     plt.xlabel('Indentation depth (m)')
376     plt.ylabel('Longitudinal resistance (h/2e2)')
377     plt.savefig('RxxSample2.svg',bbox_inches='tight', dpi = 1200)
378     #plt.figtext(.70, .63, "B = 1T")
379     #plt.figtext(.70, .58, "Scaling = 20")
380     plt.show()
381
382
383     #Simu2
384     #Variation of the potential width
385     import time
386
387     Ef = 0.15
388     V_tip = [0.05, 0.12, 0.14]
389     length_indentation = 200e-9 #Initial indentation length
390     height_indentation = 235e-9
391     #hauteursRectangle = np.linspace(0.001e-7, 0.75e-7, 300)
392     #hauteursRectangle = np.linspace(0.001e-7, 9.4e-9, 300)

```

```

393 #largeurRectangle      = 1e-7
394 widthPots              = np.linspace(1e-8, 7e-8, 300)
395 Rxxs                   = np.zeros([len(V_tip), len(widthPots)])
396 Rxys                   = np.zeros([len(V_tip), len(widthPots)])
397 Bfield = 10
398 sys = sys_builder()
399 #Gxys = np.zeros([len(Bs), 1])
400 #Gxxs = np.zeros([len(Bs), 1])
401
402 """
403 The code below is used to compute the Hall and the longitudinal resistivity. It is
404 based on a solution proposed by
405 Anton Akhmerov on the Kwant forum at the address https://www.mail-archive.com/kwant-
406 discuss@kwant-project.org/msg00110.html
407 """
408 for j, tip in enumerate(V_tip):
409     print("Tip potential: {}".format(tip))
410     for i, p in enumerate(widthPots):
411         try:
412             if i == 0:
413                 myTime = time.time()
414                 print("Width: {}".format(p))
415                 Vtip = tip
416                 sigmaTip = (p, p)
417                 #hauteurRectangle = p
418                 params = dict(Bfield=Bfield, Vg = 0)
419                 s = kwant.smatrix(sys, energy = Ef, params = params) #
420                 transmission matrix (here this)
421
422                 # First we calculate the conductance matrix given the scattering matrix S
423                 cond = np.array([[s.transmission(i, j) for j in range(n)] for i in range(
424                     n)])
425
426                 # Correct the reflection blocks, so that rows and columns sum to zero.
427                 cond -= np.diag(cond.sum(axis=0)) # a -= b means a = a-b
428
429                 # In order to calculate the nonlocal conductance we eliminate one row and
430                 one column
431                 # from the conductance matrix. This amounts to setting the corresponding
432                 voltage to zero
433                 # and using current conservation to calculate the current through the
434                 last terminal.
435                 # This is equivalent to put V_5 (lead 5) to the ground (V_5 = 0)
436                 cm = s.conductance_matrix()[:-1, :-1] #Permet de mettre un contacte à la
437                 masse, retir une ligne et une colonne
438
439                 # We then set the current to be 1 in the lead 0, -1 in lead 2, and
440                 # calculate the voltage in lead 1 (so V_3 - V_5 since V_5 = 0).
441                 Rxx = np.linalg.solve(cm, [1, -1, 0, 0])[2] #indice entre crochet ce sont
442                 les courant 1 = injecte un courant, -1 = courant qui arrive donc d'
443                 office 1 et -1. Indice 2, indice de la résistance Indice 2 = V3
444
445                 Rxxs[j][i] = Rxx
446
447                 # The same for V_4-V_5 (Hall resistance)

```

```

439     Rxy = np.linalg.solve(cm, [1, -1, 0, 0])[3] # to be completed
440     Rxys[j][i] = Rxy
441     #Gxx = 1/Rxx
442     #Gxxs[i] = Gxx
443     print('iteration', i, 'succeeded')
444     print('Resistance value', Rxx)
445 except Exception as ex:
446     print('problem encountered at iteration', i)
447     print('Warning :', ex)
448
449 finally:
450     if i == 0:
451         remainingTime = (time.time() - myTime)*len(widthPots)*(len(V_tip)-j)
452         print('Remaining time :')
453         print(time.strftime("%H:%M:%S", time.gmtime(remainingTime)))
454
455
456 plt.figure()
457
458 for index, largeurTip in enumerate(V_tip):
459     #plt.plot(Distance, Rxys[index], label = 'Rxy Vtip: {}'.format(valeurtip))
460     constriction = 30
461     RxxFinal = []
462
463     for i in range(len(Rxxs[index])):
464         RxxFinal.append(index*0.002 - Rxxs[index][i])
465
466     plt.plot(widthPots, RxxFinal, label = 'Vtip: {} eV, Constriction: {} mm'.format(
467         largeurTip, constriction))
468
469 plt.legend()
470
471 plt.legend()
472 plt.xlabel('Pontential width (m)')
473 plt.ylabel('Longitudinal resistance ( $h/2e^2$ )')
474 plt.ylim(-0.0001, 0.008)
475
476 plt.savefig('RxxSample2ComparaisonN0sansInteractionPot.svg', bbox_inches='tight', dpi
477             = 1200)
478 #plt.figtext(.70, .63, "B = 1T")
479 #plt.figtext(.70, .58, "Scaling = 20")
480 plt.show()
481
482 #Simu3
483 #Variation of the potential width for different constriction aperature
484 import time
485
486 Ef = 0.15
487 V_tip = 0.05
488 length_indentation = 200e-9 #Initial indentation length
489 height_indentations = [234e-9, 235e-9, 236e-9]
490 widthPots = np.linspace(0.15e-7, 0.65e-7, 300)
491 Rxx2s = np.zeros([len(height_indentations), len(widthPots)])
492 Rxy2s = np.zeros([len(height_indentations), len(widthPots)])

```

```

493 Bfield = 10
494
495 #Gxys = np.zeros([len(Bs),1])
496 #Gxxs = np.zeros([len(Bs),1])
497
498 """
499 The code below is used to compute the Hall and the longitudinal resistivity. It is
    based on a solution proposed by
500 Anton Akhmerov on the Kwant forum at the adress https://www.mail-archive.com/kwant-discuss@kwant-project.org/msg00110.html
501 """
502 for j, tip in enumerate(height_indentations):
503
504     print("Ouverture indentation: {}".format(tip))
505     height_indentation = tip
506     sys = sys_builder()
507
508     for i, p in enumerate(widthPots):
509         try:
510             if i == 0:
511                 myTime = time.time()
512                 print(f"{j}.{i}: Potential width: {p}")
513                 Vtip = V_tip
514                 sigmaTip = (p,p)
515                 params = dict(Bfield=Bfield, Vg = 0)
516                 s = kwant.smatrix(sys, energy = Ef, params = params) #
transmission matrix (here this)
517
518                 # First we calculate the conductance matrix given the scattering matrix S
519                 cond = np.array([[s.transmission(i, j) for j in range(n)] for i in range(
n)])
520
521                 # Correct the reflection blocks, so that rows and columns sum to zero.
522                 cond -= np.diag(cond.sum(axis=0)) # a -= b means a = a-b
523
524                 # In order to calculate the nonlocal conductance we eliminate one row and
one column
525                 # from the condutance matrix. This amounts to setting the corresponding
voltage to zero
526                 # and using current conservation to calculate the current through the
last terminal.
527                 # This is equivalent to put V_5 (lead 5) to the ground (V_5 = 0)
528                 cm = s.conductance_matrix()[:-1, :-1] #Permet de mettre un contacte à la
masse, retir une ligne et une colonne
529
530                 # We then set the current to be 1 in the lead 0, -1 in lead 2, and
531                 # calculate the voltage in lead 1 (so V_3 - V_5 since V_5 = 0).
532                 Rxx = np.linalg.solve(cm, [1, -1, 0, 0])[2] #indice entre crochet ce sont
les courant 1 = injecte un courant, -1 = courant qui arrive donc d'
office 1 et -1. Indice 2, indice de la résistance Indice 2 = V3
533
534                 Rxxs[j][i] = Rxx
535
536                 # The same for V_4-V_5 (Hall resistance)
537                 Rxy = np.linalg.solve(cm, [1, -1, 0, 0])[3] # to be completed
538                 Rxys[j][i] = Rxy

```

```

539         #Gxx = 1/Rxx
540         #Gxxs[i] = Gxx
541         print('iteration', i, 'succeeded')
542         print('Resistance value', Rxx)
543     except Exception as ex:
544         print('problem encountered at iteration', i)
545         print('Warning :', ex)
546
547     finally:
548         if i == 0:
549             remainingTime = (time.time() - myTime)*len(widthPots)*(len(
height_indentations)-j)
550             print('Remaining time :')
551             print(time.strftime("%H:%M:%S", time.gmtime(remainingTime)))
552
553
554 plt.figure()
555
556 for index, ouverture in enumerate(height_indentations):
557     #plt.plot(Distance, Rxys[index], label = 'Rxy Vtip: {}'.format(valeurtip))
558     size = W - 2*ouverture
559     stringsize = str(size)
560
561     stringSizeFinal = stringsize[0:len(stringsize) - 4]
562
563     #print(stringSizeFinal)
564     SizeFinal = float(stringSizeFinal)
565
566     lastStringNumber = stringsize[-2] + stringsize[-1]
567     #print(lastStringNumber)
568
569     lastNumber = int(lastStringNumber)
570     #print(lastNumber)
571
572     nanoSize = SizeFinal*10**(9-lastNumber)
573     #print(nanoSize)
574     plt.plot(widthPots, -Rxxs[index], label = 'Constriction aperture: {} mm'.format(
round(nanoSize, 3)))
575
576 plt.legend()
577
578 plt.xlabel('Potential width (m)')
579 plt.ylabel('Longitudinal resistance ( $h/2e^2$ )')
580 plt.ylim(0, 0.11)
581 plt.savefig('ComparaisonDeuxEdge.svg', bbox_inches='tight', dpi = 1200)
582 #plt.figtext(.70, .63, "B = 1T")
583 #plt.figtext(.70, .58, "Scaling = 20")
584 plt.show()
585
586
587 #Energy bands
588 def energy_space_longitudinal():
589     space = np.linspace(-L/2, L/2, 100)
590     Enp = np.zeros(len(space))
591     Em = np.zeros(len(space))
592     plt.figure()

```

```

593
594     for n in range(num_LL):
595         for i in range(len(space)):
596             site = kwant.builder.Site
597             site.pos = (space[i], -W/2)
598             vf = (3*t*al)/(2*h_bar)
599             Enp[i] = vf*np.sqrt(2*h_bar*e)*np.sqrt(n*Bfield) + onsite(site)#
to be completed
600             Enm[i] = -vf*np.sqrt(2*h_bar*e)*np.sqrt(n*Bfield) + onsite(site)
601
602         if n == 0:
603             plt.plot(space, Enp, 'r', label = 'LL: 0')
604             plt.legend()
605
606         else:
607             plt.plot(space, Enp, 'b')
608             plt.plot(space, Enm, 'b')
609
610     plt.plot(space, Ef*np.array([1 for i in range(len(space))]), 'r-')
611     plt.ticklabel_format(style='sci', axis='x', scilimits=(0,0))
612     plt.xlabel('Longitudinal position for y = 0 (m)')
613     plt.ylabel('Energy (eV)')
614     plt.savefig('LongitudinalEnergyN0PAsCroisement.svg', bbox_inches='tight', dpi =
1200)
615     plt.show()
616
617 Ef = 0.15
618 Vtip = 0.12
619 Bfield = 10
620 energy_space_longitudinal()
621
622
623 def energy_space_transversal():
624     space = np.linspace(-W/2, W/2, 100)
625     Enp = np.zeros(len(space))
626     Enm = np.zeros(len(space))
627     plt.figure()
628
629     for n in range(num_LL):
630         for i in range(len(space)):
631             site = kwant.builder.Site
632             site.pos = (0, space[i])
633             vf = (3*t*al)/(2*h_bar)
634             Enp[i] = vf*np.sqrt(2*h_bar*e)*np.sqrt(n*Bfield) + onsite(site)# to
be completed
635             Enm[i] = -vf*np.sqrt(2*h_bar*e)*np.sqrt(n*Bfield) + onsite(site)
636         if n == 0:
637             plt.plot(space, Enp, 'r', label = 'LL: 0')
638             plt.legend()
639
640         else:
641             plt.plot(space, Enp, 'b')
642             plt.plot(space, Enm, 'b')
643
644     plt.plot(space, Ef*np.array([1 for i in range(len(space))]), 'r-')
645     plt.ticklabel_format(style='sci', axis='x', scilimits=(0,0))

```

```
646 plt.xlabel('Transversal position for x = 0 (m)')
647 plt.ylabel('Energy (eV)')
648 #plt.savefig('transversal-L400e-9-H0,75e-7-Ef0,07-V0,05-sigma2e-7.svg',
649             bbox_inches='tight', dpi = 1200)
650 plt.show()
651 energy_space_transversal()
```

7.2.3 InGaAs code

This section presents code lines corresponding to the results in [5](#)

```
1
2 import kwant
3 import scipy
4 import numpy as np
5 from matplotlib import pyplot as plt
6 from types import SimpleNamespace
7
8
9 h = 6.626069e-34 # Planck constant (Js)
10 e = 1.602e-19 # electron charge (C)
11 c = 299792458 # Light celerity (m/s)
12 kB = 1.3806503e-23 # Boltzmann constant (kg m2/Ks2)
13 m_e = 9.1e-31 # electron mass (kg)
14 h_bar = h/(2*np.pi)
15
16
17 asquare = 0.4225e-9 # [m] a is the lattice parameter
18 tsquare = 1 # [eV] t is the hopping parameter
19
20 scaling = 8 # scaling factor
21
22 """scaling"""
23
24 a = asquare * scaling
25 t = tsquare / scaling**2
26 print("Max value Ef: {} eV".format(t*0.5))
27
28
29 #Basic system's parameters
30 W = 500e-9 ; L = 700e-9 # width and length of the electronic system
31
32 width_leads = 30e-9 # width of the small leads of the Hall bar
33 posL = 200e-9 # pos of the leads along x
34 #posL = 4e-7
35 lead_ext = posL + width_leads/2
36 lead_int = posL - width_leads/2
37
38 #Indentation's parameters
39 height_indentation = 125e-9
40 length_indentation = 200e-9
41 position_indentation1 = (0, -W/2)
```

```

42 position_indentation2 = (0, W/2)
43
44 #Potential parameters
45 #sigma = (7.458e-8, 7.458e-8)
46 #sigma = (7.4072e-8, 7.4072e-8)
47 sigma = (8e-8, 9e-8)
48
49 sigma1 = (6e-8, 7e-8)
50 Vtip1 = 0.01
51 center = (0,0)
52
53
54 def geom(pos):
55     x, y = pos
56     x_indentation1, y_indentation1 = position_indentation1 #Position of the bottom
indentation
57     x_indentation2, y_indentation2 = position_indentation2 #Posistion of the top
indentation
58
59     #Parameters of the bottom indentation
60     m1_indentation1 = 2*height_indentation/length_indentation
61     p1_indentation1 = y_indentation1 + height_indentation*(1-2*x_indentation1/
length_indentation)
62     m2_indentation1 = -m1_indentation1
63     p2_indentation1 = y_indentation1 + height_indentation*(1+2*x_indentation1/
length_indentation)
64
65     #Parameters of the top indentation
66     m1_indentation2 = m2_indentation1
67     p1_indentation2 = y_indentation2 + height_indentation*(-1+2*x_indentation2/
length_indentation)
68     m2_indentation2 = -m1_indentation2
69     p2_indentation2 = y_indentation2 - height_indentation*(1+2*x_indentation2/
length_indentation)
70
71     #Drawing of the bottom indentation
72     if x_indentation1 - length_indentation/2 < x < x_indentation1 and y_indentation1
< y < m1_indentation1*x + p1_indentation1:
73         return False
74     if x_indentation1 <= x < x_indentation1 + length_indentation/2 and y_indentation1
< y < m2_indentation1*x + p2_indentation1:
75         return False
76
77     #Drawing of the top indentation
78     if x_indentation2 -length_indentation/2 < x < x_indentation2 and m1_indentation2*
x + p1_indentation2 < y < y_indentation2:
79         return False
80     if x_indentation2 <= x < x_indentation2 + length_indentation/2 and
m2_indentation2*x + p2_indentation2 < y < y_indentation2:
81         return False
82
83     elif -L/2 < x < L/2 and -W/2 < y < W/2:
84         return True
85
86     else:
87         return False

```

```
88
89
90 def lead_shape(pos):
91     x, y = pos
92     return -W/2 < y < W/2
93
94 def lead_shape_left(pos):
95     x, y = pos
96     return -lead_ext < x < -lead_int
97
98 def lead_shape_right(pos):
99     x, y = pos
100    return lead_ext > x > lead_int
101
102
103 def gauss(site, center, sigma, amplitude):
104     x, y = site.pos
105     x0, y0 = center
106     sigmax, sigmay = sigma
107
108     return amplitude*np.exp(-((x - x0)**2)/(2*sigmax**2) - ((y - y0)**2)/(2*sigmay
109     **2))
110
111 def onsite(site):
112     return Vg + 4*t + gauss(site, center, sigma, Vtip) - gauss(site, center, sigma1,
113     Vtip1)
114
115 def hopping(site_i, site_j):
116     xi, yi = site_i.pos
117     xj, yj = site_j.pos
118
119     """ Change the definition of hop to include the magnetic field Bfield in the
120     definition of the hopping parameter """
121
122     hop = t*np.exp(np.pi*1j*e*Bfield*(yi+yj)*(xj-xi)/h)
123
124     return hop
125
126 def sys_builder():
127     lat = kwant.lattice.square(a, norbs = 1) # norbs gives the number of orbitals per
128     atom. It is needed to compute J
129
130     sys = kwant.Builder() # construction of the system
131     sys[lat.shape(geom, (0,0))] = onsite # The onsite functions is given in argument
132
133     sys[lat.neighbors()] = hopping # the hopping function is given in argument
134
135     """ Lead 1 """
136     sym0 = kwant.TranslationalSymmetry(lat.vec((-1, 0)))
137     lead0 = kwant.Builder(sym0)
138     lead0[lat.shape(lead_shape, (0, 0))] = 4*t
139     lead0[lat.neighbors()] = hopping
```

```

140 """ Lead 2 """
141 sym1 = kwant.TranslationalSymmetry(lat.vec((1, 0)))
142 lead1 = kwant.Builder(sym1)
143 lead1[lat.shape(lead_shape, (0, 0))] = 4*t
144 lead1[lat.neighbors()] = hopping
145
146 """ Lead 5 """
147 sym4 = kwant.TranslationalSymmetry(lat.vec((0, 1)))
148 lead4 = kwant.Builder(sym4)
149 lead4[lat.shape(lead_shape_left, (-posL, 0))] = 4*t
150 lead4[lat.neighbors()] = hopping
151
152 """ Lead 3 """
153 #sym2 = kwant.TranslationalSymmetry(graphene.vec((0, 1)))
154 lead2 = kwant.Builder(sym4)
155 lead2[lat.shape(lead_shape_right, (posL, 0))] = 4*t
156 lead2[lat.neighbors()] = hopping
157
158 """ Lead 4 """
159 sym3 = kwant.TranslationalSymmetry(lat.vec((0, -1)))
160 lead3 = kwant.Builder(sym3)
161 lead3[lat.shape(lead_shape_left, (-posL, 0))] = 4*t
162 lead3[lat.neighbors()] = hopping
163
164
165
166
167
168
169
170 """ The leads are attached """
171 sys.attach_lead(lead0)
172 sys.attach_lead(lead1)
173 sys.attach_lead(lead2)
174 sys.attach_lead(lead3)
175 sys.attach_lead(lead4)
176
177 sys = sys.finalized()
178
179 return sys
180 #### Schematic of the Hall bar ####
181
182
183
184 #
185 # ,-----o-----Vxx-----.
186 # | Lead 3 | | | Lead 5 |-----'---'---'---' (ground)
187 # Vxy    ___| |_____| |___
188 # |      I
189 # | Lead 1  -----> Lead 2
190 # |      ___| |_____| |___
191 # | Lead 4 | | | not implemented (because not necessary)
192
193
194 sys = sys_builder()
195

```

```

196 def poltsys():
197     kwant.plot(sys, site_size = 1e-9)
198
199 #poltsys()
200
201
202 Ef = 0.066
203 if Ef > 0.5*t:
204     print('\033[31m' + "Warning, Ef is too high !")
205     print('\033[0m')
206
207
208 #Bfield = (2*Ef**2*h_bar)/(9*t**2*a**2*e*0.5) # to be completed
209 Bfield = 6
210
211 """ Parameter for the zero density zone """
212 Vg      = 0
213 Vtip     = 0.015
214 params  = dict(Bfield=Bfield, Vg = Vg) # params take the magnetic field as a
215     parameter for the function hopping
216
217
218 """ The wavelength must be (much more) larger than the lattice parameter """
219 lambda_F = 2 * np.pi * a * np.sqrt(t / Ef) # computation of the wavelength
220 if lambda_F/a < 2:
221     print('Warning : lambda_F must be larger than the lattice parameter a')
222
223
224 num_LL = 5
225
226 plt.figure()
227
228 for n in range(num_LL):
229     """
230     Change the definition of En to calculate the Landau levels energy as a function
231     of
232     the magnetic field Bfield and the Landau level label n
233     """
234     m = h_bar**2 / (2*a**2*t)
235     En = h_bar * e * Bfield * (n + 0.5)/m # to be completed
236     #print(En)
237
238     x = np.array([0, 1]) ; y = En*np.array([1, 1]) # in order to plot the Landau
239     levels
240     plt.plot(x, y, 'b')
241
242 plt.plot(x, Ef*np.array([1, 1]), 'r-') # to plot the Fermi energy (in red)
243
244 plt.xlabel('DOS (a.u.)')
245 plt.ylabel('Energy (eV)')
246
247 plt.show()
248

```

```

249 Vtip = 0.014
250 Vtip1 = 0.013
251 vals=[onsite(sys.sites[n]) for n in range(sys.graph.num_nodes)]
252 kwant.plotter.map(sys, vals, cmap = 'RdBu')
253
254
255 #para = np.linspace(7.2e-8,7.25e-8,10)
256 para = [5, 5.7, 6, 6.5, 6.9]
257 Ef = 0.01
258 Vtip = 0.01
259 Vtip1 = 0.007
260 #Bfield = 3.2
261 for i, w in enumerate(para):
262     #center = (0, w)
263     #sigma = (w,w)
264     #sys = sys_builder()
265     Bfield = w
266     wfs = kwant.wave_function(sys, energy=Ef, params = params) # the wave function is
267                                     # parameters in
268     scattering_wf = wfs(0) # all scattering wave functions from lead 0
269     J0 = kwant.operator.Current(sys)
270     wf_left = wfs(0)
271
272     current = sum(J0(p, params = params) for p in wf_left) # to sum over all the lead
273     's mode
274
275     kwant.plotter.current(sys, current, cmap='viridis')
276
277 #Simul
278 #Variation of the magnetic field
279 import time
280
281 Ef = 0.01
282 V_tip = [0.014]
283 Vtip1 = 0.013
284 Bfields = np.linspace(7,11, 600)
285 Rxxs = np.zeros([len(V_tip),len(Bfields)])
286 Rxys = np.zeros([len(V_tip),len(Bfields)])
287 sys = sys_builder()
288 #Gxys = np.zeros([len(Bs),1])
289 #Gxxs = np.zeros([len(Bs),1])
290
291 """
292 The code below is used to compute the Hall and the longitudinal resistivity. It is
293 based on a solution proposed by
294 Anton Akhmerov on the Kwant forum at the adress https://www.mail-archive.com/kwant-discuss@kwant-project.org/msg00110.html
295 """
296 for j, tip in enumerate(V_tip):
297     print("Tip: {}".format(tip))
298
299     for i, s in enumerate(Bfields):

```

```

300     try:
301         if i == 0:
302             myTime = time.time()
303             print(s)
304             Vtip = tip
305             Bfield = s
306             params = dict(Bfield=Bfield, Vg = 0)
307             s = kwant.smatrix(sys, energy = Ef, params = params) #
transmission matrix (here this)
308
309             # First we calculate the conductance matrix given the scattering matrix S
310             cond = np.array([[s.transmission(i, j) for j in range(n)] for i in range(
n)])
311
312             # Correct the reflection blocks, so that rows and columns sum to zero.
313             cond -= np.diag(cond.sum(axis=0)) # a -= b means a = a-b
314
315             # In order to calculate the nonlocal conductance we eliminate one row and
one column
316             # from the conductance matrix. This amounts to setting the corresponding
voltage to zero
317             # and using current conservation to calculate the current through the
last terminal.
318             # This is equivalent to put V_5 (lead 5) to the ground (V_5 = 0)
319             cm = s.conductance_matrix()[:-1, :-1] #Permet de mettre un contacte à la
masse, retir une ligne et une colonne
320
321             # We then set the current to be 1 in the lead 0, -1 in lead 2, and
322             # calculate the voltage in lead 1 (so V_3 - V_5 since V_5 = 0).
323             Rxx = np.linalg.solve(cm, [1, -1, 0, 0])[2] #indice entre crochet ce sont
les courant 1 = injecte un courant, -1 = courant qui arrive donc d'
office 1 et -1. Indice 2, indice de la résistance Indice 2 = V3
324
325             Rxxs[j][i] = Rxx
326
327             # The same for V_4-V_5 (Hall resistance)
328             Rxy = np.linalg.solve(cm, [1, -1, 0, 0])[3] # to be completed
329             Rxys[j][i] = Rxy
330             #Gxx = 1/Rxx
331             #Gxxs[i] = Gxx
332             print('iteration', i, 'succeeded')
333             print('Resistance value', Rxx)
334         except Exception as ex:
335             print('problem encountered at iteration', i)
336             print('Warning:', ex)
337
338     finally:
339         if i == 0:
340             remainingTime = (time.time() - myTime)*len(Bfields)*(len(V_tip)-j)
341             print('Remaining time:')
342             print(time.strftime("%H:%M:%S", time.gmtime(remainingTime)))
343
344
345     plt.figure()
346
347     for index, valeurtip in enumerate(V_tip):

```

```

348 #plt.plot(Distance , Rxys[index], label = 'Rxy Vtip: {}'.format(valeurtip))
349 plt.plot(Bfields , -Rxxs[index])
350
351 #plt.legend()
352
353 plt.xlabel('Magnetic field (T)')
354
355 plt.ylabel('Longitudinal resistance ( $h/2e^2$ )')
356 plt.ylim(-0.01, 1)
357 #plt.savefig('RxxBSupplementInGaAS.svg',bbox_inches='tight', dpi = 1200)
358 #plt.figtext(.72, .8, "B = 8T")
359 #plt.figtext(.72, .75, "Scaling = 8")
360 plt.show()
361
362
363 def energy_space_longitudinal(Fermi):
364     space = np.linspace(-L/2, L/2, 100000)
365     En = np.zeros(len(space))
366
367     plt.figure()
368
369     for n in range(num_LL):
370         for i in range(len(space)):
371             site = kwant.builder.Site
372             site.pos = (space[i], 0)
373             m = h_bar**2 / (2*a**2*t)
374             En[i] = h_bar * e * Bfield * (n + 0.5)/m + onsite(site) - 4*t # to be
completed
375
376
377         if En[i] > Fermi - 0.000001*Fermi and En[i]<Fermi +0.000001*Fermi:
378             print("rayon : ", space[i])
379             print("surface : ", np.pi*space[i]**2)
380
381         if n == 0:
382             plt.plot(space,En,'r', label = 'LL: 0')
383             plt.legend()
384
385         else:
386             plt.plot(space,En,'b')
387
388
389     plt.plot(space, Ef*np.array([1 for i in range(len(space))]), 'r-')
390     plt.ticklabel_format(style='sci', axis='x', scilimits=(0,0))
391     plt.xlabel('Longitudinal position for y = 0 (m)')
392     plt.ylabel('Energy (eV)')
393     #plt.savefig('EnergyInGaAsB9.svg',bbox_inches='tight', dpi = 1200)
394     plt.show()
395
396
397 Bfield = 10
398 Ef = 0.01
399 Vtip = 0.004
400 Vtip1 = 0.003
401 energy_space_longitudinal(Ef)
402

```

```
403
404 def energy_space_transversal(Fermi):
405     space = np.linspace(-W/2, W/2, 100000)
406     En = np.zeros(len(space))
407
408     plt.figure()
409
410     for n in range(num_LL):
411         for i in range(len(space)):
412             site = kwant.builder.Site
413             site.pos = (0, space[i])
414             m = h_bar**2 / (2*a**2*t)
415             En[i] = h_bar * e * Bfield * (n + 0.5)/m + onsite(site) - 4*t # to be
completed
416
417
418             if En[i] > Fermi - 0.000001*Fermi and En[i]<Fermi +0.000001*Fermi:
419                 print("rayon : ", space[i])
420                 print("surface : ", np.pi*space[i]**2)
421
422         if n == 0:
423             plt.plot(space,En,'r', label = 'LL: 0')
424             plt.legend()
425
426         else:
427             plt.plot(space,En,'b')
428
429
430     plt.plot(space, Ef*np.array([1 for i in range(len(space))]), 'r-')
431     plt.ticklabel_format(style='sci', axis='x', scilimits=(0,0))
432     plt.xlabel('Transversal position for x = 0 (m)')
433     plt.ylabel('Energy (eV)')
434     plt.savefig('EnergyInGaAsB9,5.svg',bbox_inches='tight', dpi = 1200)
435     plt.show()
436
437 Bfield = 9.7
438 Ef = 0.01
439 Vtip = 0.014
440 Vtip1 = 0.013
441 energy_space_transversal(Ef)
```

UNIVERSITÉ CATHOLIQUE DE LOUVAIN
École polytechnique de Louvain

Rue Archimède, 1 bte L6.11.01, 1348 Louvain-la-Neuve, Belgique | www.uclouvain.be/epl