Electronic properties of graphene in inhomogeneous magnetic fields

Elektronische eigenschappen van grafeen in inhomogene magnetische velden

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Massoud Ramezani Masir

Promoter:
Prof. Dr. François Peeters

Antwerpen

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Members of the Jury:

**Chairman**
Prof. Dr. J. Tempere, Universiteit Antwerpen, Belgium

**Promotor**
Prof. Dr. François Peeters, Universiteit Antwerpen, Belgium

**Members**
Prof. Dr. E. De Wolf, Universiteit Antwerpen, Belgium
Prof. Dr. J. Verbeeck, Universiteit Antwerpen, Belgium
Prof. Dr. D. Lamoen, Universiteit Antwerpen, Belgium
Prof. Dr. Ph. Lambin, University of Namur, Belgium
Prof. Dr. A. Matulis, Center of Physical Sciences and Technology, Vilnius, Lithuania

**Contact Information**
Massoud Ramezani Masir
Universiteit Antwerpen
Departement Fysica
Groenenborgerlaan 171
2020 Antwerpen
Belgium
mrmphys@gmail.com
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Massoud Ramezani Masir
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1

Introduction

1.1 The carbon atom and its allotropes

Carbon and its allotropes and components are widely spread in our universe. There is no material as important as carbon to our life. It is in the food we eat, the clothes we wear, the cosmetics we use and the gasoline that fuels our cars. Its name comes from the Latin world carbo for coal and charcoal. Carbon compounds can resist in difficult ambient conditions due to its strong and stable bonds to itself. This makes carbon an important element to form long chains and rings of atoms, which are the basis structure for many compounds that contain the living cells, such as DNA.

Carbon is one of the most flexible elements in terms of the number of compounds it may form. This capability is due to the types of bonds it can form and the number of different elements it can join in bonding. Carbon belongs to group fourteen on the periodic table and has four electrons available to form covalent bonds and its ground state configurations is $1s^2, 2s^2 2p^2$. There are four electrons on orbitals $2s$ and $2p$ with two possible configuration shown in Fig. 1.1. As the $2p$ orbitals ($2p_x, 2p_y$, and $2p_z$) are roughly 4 eV higher in energy than the $2s$ orbital, it is energetically favorable to put 2 electrons in the $2s$ orbital and only 2 of them in the $2p$ orbitals. In the presence of some atoms, such as e.g. H, O, or other C atoms, in order to have covalent bonds it is better to excite one electron from the $2s$ to the third $2p$ orbital. This kind of hybridization is called $sp^2$ hybridization in which, two of the $2p$-orbitals and one $2s$-orbital take part in the hybridization process. This hybridization forms three equivalent $sp^2$-hybrid orbitals, which adopt a trigonal planar geometry, and one unchanged $p$-orbital that lies at right angles to the plane of the hybrid orbitals, as shown schematically in Fig. 1.2.

Carbon itself has a very short life time and can only be stabilized in various multi-atomic structures with different molecular configurations called allotropes. Some well-known allotropes of carbon are shown in Fig. 1.3: graphite, diamond and fullerenes which also include buckyballs, carbon nanotubes, carbon nanobuds and nanofibers. In the next section we introduce briefly diamond, graphite and
Fullerene as three well-known allotrops of carbon:

1.1.1 Diamond

Diamond is the most famous allotrope of carbon. Each carbon atom in diamond is bonded to four other partner carbons in a tetrahedron with equivalent $sp^3$-bonds in which the $2s$ orbital mixes with the three $2p$ orbitals to form four $sp^3$ hybrids. A tetrahedron is composed of four triangular faces, three of which meet at each vertex. The tetrahedral arrangement of atoms is the source of many of diamond’s properties. Diamond has a low electrical conductivity, the highest thermal conductivity, highly transparent, excellent insulator due to its large band gap in its electronic spectrum and it is among the hardest materials known. Industrially it can be used for cutting, drilling, grinding, and polishing. There is no natural substance that one can use to cut or scratch a diamond, except diamond itself.

1.1.2 Graphite

Graphite is one of the most common allotropes of carbon. In graphite each carbon atom is covalently bonded to three carbon atoms to give trigonal geometry. Each carbon atom in graphite is $sp^2$ hybridized. Three out of four valence electrons of each carbon atom are used in bond formation with three other carbon atoms while the fourth electron is free to move in the structure of graphite. It is the most stable allotrope of carbon. At very high temperatures and pressures (roughly 2000°C and 5 GPa), it can be transformed into diamond and at around 700°C in the presence of oxygen it forms carbon dioxide. Unlike diamond, graphite is a very good conductor.
1.2. GRAPHENE

Figure 1.2: $sp^2$ hybridization and forming a $\pi$ bond from two $p$ orbitals.

and it is very soft a property that is in pencils for writing.

1.1.3 Fullerene

Fullerenes are molecules build up from carbon atoms, which were first discovered in 1985 by researchers at Rice University. They have different forms, such as hollow sphere, ellipsoid, or tube. Spherical fullerenes are also called buckyballs and cylindrical ones are called carbon nanotubes or buckytubes. From the structural point of view fullerenes are similar to graphite, with hexagonal carbon ring but they may also contain pentagonal or heptagonal rings. In the past decades the discovery of nanotubes and fullerenes attracted a lot of attention among physicists and chemists. In 1996 the Nobel Prize in Chemistry was awarded jointly to Robert F. Curl Jr., Sir Harold W. Kroto and Richard E. Smalley for their discovery of fullerenes.

1.2 Graphene

Graphene is an allotrope of carbon, whose structure is a single layer of hexagonal arrangement of $sp^2$-bonded carbon atoms [2]. This name was first given in Ref. [3] to describe a single layer of graphite as one of the components of graphite.

For a long time, one was convinced that two dimensional crystals can not exist because thermal fluctuations [4–8] will destroy it. A lot of effort in the past to
create atomically thin films of other materials failed since the films became unstable and tended to separate and clump up rather than form perfect layers. It came on a big surprise when in 2004 a group of scientists in Manchester university led by Andre Geim and Kostya Novoselov succeeded to extract a stable single layer of carbon atoms. Nowadays the stability of graphene is explained by postulating small out-of-plane corrugations [9, 10].

The method used by the Manchester group to extract a single layer of Graphite was simple. Graphite consists of several graphene layers coupled to each other by weak van der Waals-bonding. They extracted a single layer of graphene using micromechanical exfoliation or, simply, the Scotch tape technique. This technique consists of repeated peeling of multilayered graphite of a highly ordered pyrolytic graphite (HOPG) crystal with a cellophane tape and, then pressing the tape on a Si/SiO\textsubscript{2} substrate to deposit the graphene samples. The sample sizes produced in this way is of the order of several \(\mu m^2\). In fact, when you are writing with a pencil, if you look at the results under the microscope probably you will see one of these sheets has to be a single layer thick.

After extracting a single layer of graphene from graphite, the Manchester researchers transferred this graphene sheets onto thin SiO\textsubscript{2} on a silicon wafer in
1.3. GRAPHENE APPLICATIONS

order to make graphene electrically isolated. Since $SiO_2$ was weakly interacting with the graphene, this process can provide nearly charge-neutral graphene layers. Using the doped silicon under the $SiO_2$ let them use it as a back gate electrode to change the charge density in the graphene layer. This process led to the first observation of the anomalous Hall effect in graphene by Geim and Novoselov [11] and later by Philip Kim and Yuanbo Zhang [12] in 2005. These experiments demonstrate the theoretically predicted $\pi$ Berry’s phase of massless Dirac fermions in graphene.

In 1947 P. R. Wallace studied theoretically a single layer of graphite [13]. His purpose was to understand the electronic properties of 3D graphite. Later in 1984 Semenoff considered graphene in a magnetic field as an analog of $(2 + 1)$-dimensional electrodynamics in order to describe anomaly in such systems. Semenoff obtained the Landau levels of this system and especially the Landau level precisely at the Dirac point. This level is responsible for the anomalous integer quantum Hall effect [11, 12].

Geim and Novoselov received several awards for their pioneering research on graphene, including: the Mott medal for Geim in 2007 for the discovery of a new class of materials free-standing two-dimensional crystals in particular graphene, the 2008 EuroPhysics Prize for discovering and isolating a single free-standing atomic layer of carbon (graphene) and elucidating its remarkable electronic properties, and Körber Prize for Geim in 2009 for developing the first two-dimensional crystals made of carbon atoms. And On October 5, 2010, the Nobel Prize in Physics was awarded to Andre Geim and Konstantin Novoselov from the University of Manchester for their work for groundbreaking experiments regarding the two-dimensional material graphene.

1.3 Graphene applications

Graphene with its remarkable properties can open a new way of thinking to invent new applications in transparent electronics, in flexible electronics and electronics that are much faster than those available today. Graphene can also be used outside digital applications, for instance: using graphene as ultra-sensitive detectors that could recognize diseases like cancer faster than current tests. Another possible application could be adding graphene powder to tyres to make them stronger. About 200 companies are now involved in research related to graphene. The benefits to both businesses and to the consumer are obvious: faster and cheaper devices which are thinner and flexible. Graphene is one of the strongest material ever measured, with a Young’s modulus of about 1 TPa. Graphene is some 200 times stronger than structural steel. It would take an elephant, balanced on a pencil, to
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Figure 1.4: (a) SEM images of graphite plates on the Si(001) substrate [14]. (b) Atomic force microscopy image of a graphene crystal on top of an oxidized Si substrate [2, 15]. (c) Illustration for the Scotch tape technique. (D) STM topographic images of different regions of the graphene flake which a honeycomb structure is observed. [16].

break through a sheet of graphene the thickness of Saran Wrap [17](Fig. 1.7). A comparison between superlative mechanical, thermal and electronic properties of graphene with other materials are given by Ref. [18] in Fig. 1.5. The amazing properties of Graphene attracted lots of attention between scientists all around the world. Fig. 1.6 shows the contribution of different countries and the number of published papers up to 2010 [18]).

1.3.1 Graphene photodetector

To compare with other materials, electrons and holes move much faster in graphene. Unlike group III-V semiconductors such as $GaAS$, $GaSb$, $InSb$, etc, graphene absorbs light over a wide range of wavelengths, from the visible to the infrared.

Recently at IBM a group led by Phaedon Avouris, used internal electric field by placing palladium or titanium (see Fig. 1.8) electrodes on top of a piece of multilayered or single-layered graphene in order to separate electron-hole pairs and overcome the problem of recombination [19,20]. The metal contacts produce elec-
tric fields at the interface between the electrodes and graphene. This electrical field separates the electrons and holes efficiently, and when one shines light a photocurrent is produced. The advantage of this setup is that, there is no need to apply a bias voltage, which can produce unwanted noise. The graphene photodetector can achieve error-free detection of optical data streams at rates of 10 Gbit/s. The IBM team is still working on optimizing the photodetector’s operation and combining it with other optical devices. The graphene photodetector would be particularly competitive in the long wavelength range of the electromagnetic spectrum and for ultrafast measurements [20].
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Figure 1.6: Contribution of different countries in research on graphene and the number of published papers up to 2010. (Figures are from Ref: [18])

1.3.2 Gas sensors

Before using graphene as a gas sensor the best gas sensors were solid-state gas sensors [23, 24]. The limit of these devises is the thermal fluctuation due to the thermal motion of charges and defects which result in intrinsic noise several orders of magnitudes larger than the signal from individual molecules. In 2007 it was shown that [25] gas molecules attach or detach on graphene’s surface affect its electronic properties in a measurable way. In fact, it is possible to measure the effect of a single molecule bonded to graphene since it can change the local carrier concentration in graphene and lead to changes in resistance. This means that it is possible to create gas sensors which are sensitive to a single molecule. The secret of this high sensitivity is from the fact that graphene is electronically an exceptional low-noise material, which makes it a promising candidate for chemical detectors.

1.3.3 LCD and flexible screen

High optical transparency, atomic layer thickness, low resistivity, and high chemical stability makes graphene an ideal candidate for transparent electrodes in various optoelectronic devices. Plastic can become conductive by adding only 1% of graphene while it will remain transparent. This property can be used in devices such as mobile phones, TVs and touchscreen. The current technology used in these devices is based on thin metal-oxide films with Indium. Indium is very expensive and its supply is expected to be finished in just 10 years. Therefore researchers are looking for new conductive transparent films as a replacement.

In 2008 Geim and his research group in Manchester demonstrated that graphene can be used as conducting transparent thin films which can be used as electrodes
1.3. GRAPHENE APPLICATIONS

in LCDs and other photonic devices [21]. Over a very large range of wavelengths, graphene absorbs only 2.3% of light. An LCD consists of a liquid-crystal material with two transparent electrodes replaced on top and bottom as shown in Fig. 1.9(a). With changing voltage over the two electrodes the polarized light can pass through the stack or be blocked (see Fig. 1.9(b)). We can use this property to selectively turn pixels on and off.

Samsung is one of the biggest investors on graphene research who wants to use it in electronic technology. Recently in January 2011 they demonstrated a 4.5-inch flexible AMOLED (active-matrix organic light-emitting diode) that was just 0.33 mm thick by using graphene (see Fig. 1.9). Probably we will see soon the first flexible smart phone or tablet with graphene by Samsung.

1.3.4 Spintronics

Spin electronics is looking for an answer to the question: How can we control and manipulate the spin degrees of freedom? In spintronic devices information is processed by using electron spins, and the strong research interest in it originates from the fact that it promises to be smaller, more adaptable, and faster than today’s electronic devices [27]. Graphene is a very promising material for spintronic devices because its electron spin can maintain its direction for a long time and, as a result, information can be stored and coherent quantum manipulation should be realizable over long times. Several potential applications of spintronics could be spin-field-effect transistor (spin-FET) [28], spin-light emitting diode (spin-LED) [29],...
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Figure 1.8: (Figures from Refs. [19,20]) (a) A 3-dimensional schematic view of the metal-graphene-metal photodetector. (b) The total photocurrent generated. (c) Relative photoresponse as a function of the light intensity modulation frequency. 3-dB bandwidth of this metal-semiconductor-metal photodetector is about 16 GHz. Inset: the receiver eye-diagram obtained using this metal-semiconductor-metal photodetector. A completely open eye is obtained and error-free optical signal detection is demonstrated.

magneto resistive random access memory (MRAM) [30], etc.

1.3.5 High speed transistors

Other companies like IBM and Nokia have also been involved in graphene research for electronic devices. Recently IBM presented a field-effect transistor (FET) fabricated on a 2-inch graphene wafer [22] (see Fig. 1.10) and inferred 100 GHz transistor operation which is already comparable with the fastest silicon-based transistors which runs at about 40 GHz. Later another group of researchers from UCLA reported the fabrication of the highest speed graphene transistors, with a cutoff frequency up to 300 GHz [26].
1.4. MOTIVATION AND OUTLINE

Figure 1.9: (a) Schematic illustration of LCD based on graphene. (b) Normalized transmission for LCD built using graphene instead of the commonly used indium tin oxide for one of its electrodes. (Figures from Ref. [21]) (c) Samsung Graphene-Based touch screen.

1.4 Motivation and Outline

One of the biggest dreams for graphene is to use it one day as a replacement of silicon. But the biggest obstacle is that graphene itself does not have a band gap. This property makes graphene always conducting and conduction cannot be completely turned off. One of the most challenging tasks is to learn how to control the electron behavior using electric fields in this two-dimensional (2D) layer. This task is complicated by the so-called Klein effect according to which Dirac electrons in graphene can tunnel through any electric barrier [31, 32].

In my thesis, I wanted to learn (and to propose mechanisms) "How to control the electron motion in graphene?". The second motivation was to investigate if it is possible to use nonhomogeneous magnetic fields to open a gap in the energy spectrum of graphene. In order to tackle these questions, I approached the problem in three different directions:
• **Inhomogeneous magnetic fields:** An alternative approach to control the motion of electrons is to use non homogeneous magnetic fields which was previously realized successfully in GaAs heterostructures. Such nonhomogeneous magnetic fields can be created e.g. through the deposit of nanostructured ferromagnets [33] or applying in-plane and out of plane strain [34]. During my PhD I investigated several model problems for which I studied energy levels, transmission and scattering of electrons for different types of inhomogeneous magnetic fields such as magnetic step, single and multiple magnetic barriers and magnetic dot. In order to do so, I solved the effective Dirac equation for a single electron in graphene in the presence of different magnetic field profiles.

• **Opening a gap:** As a proof of concept I introduced a Kronig-Penney model composed of periodic magnetic and potential barriers. The band structure of this periodic system was obtained semi-analytically and I investigated which are the conditions (i.e. model parameters) needed to open a gap. As a bonus
1.4. MOTIVATION AND OUTLINE

Figure 1.11: (a) Schematic of the three-dimensional view of the device layout. D, drain; G, gate; S, source. (b) Schematic of the cross-sectional view of the device. In this device, the $Co_2Si-Al_2O_3$ core-shell nanowire defines the channel length, with the 5-nm $Al_2O_3$ shell functioning as the gate dielectrics, the metallic $Co_2Si$ core functioning as the self-integrated local gate and the self-aligned platinum thin-film pads functioning as the source and drain electrodes. (c) SEM images of a graphene transistor with a self aligned nanowire gate. (d) Measured small signal current gain $|h_{21}|$ as a function of frequency $f$ at $V_{ds} = -1$ V for a gate length, 144 nm. (Figures are from Ref. [26])

I show that electrons can be collimated in such structures.

- **Localized solutions:** The ultimate control of electron motion is the ability to realize spatial localization. The solution of the Dirac equation with an inhomogeneous profile was considered by using the analogy with optics called the Gaussian beam techniques which was introduced before to describe electro-magnetic beams such as laser beams.

The thesis is organized as follows:

- **Chapter 2:** In the whole thesis the Dirac equation is solved for electrons around the $K$ point in the presence of different inhomogeneous structures. In order to motivate the use of the Dirac equation for an electron in graphene and what are the conditions and limitations in the presence of magnetic
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fields, I review in this chapter some of the most important electronic properties of graphene. I discuss in detail the tight binding model for single layer graphene, the effective Dirac Hamiltonian, the electron spectrum in a magnetic field, and I briefly discuss how to realize experimentally inhomogeneous magnetic fields.

- **Chapter 3**: Using the Gaussian beam technique from beam optics I calculate the electron transmission through simple non-homogeneous structures, such as flat and bent p-n junctions and superlattices.

- **Chapter 4**: The Fabry-Pérot resonances of a potential barrier profile in graphene is investigated. The effect of a perpendicular magnetic field on such resonances is studied numerically in detail.

- **Chapter 5**: In order to be able to confine the electron and to understand how we can control the electron motion using inhomogeneous magnetic fields we study in this chapter the transmission and bound states for an electron in single layer graphene in the presence of magnetic steps, and single and multiple magnetic barriers.

- **Chapter 6**: I generalized the calculations of chapter 5 to the case of electron motion in bilayer graphene.

- **Chapter 7**: In order to realize the opening of a gap in the band structure of graphene. I investigated the properties of Dirac electrons in a magnetic superlattice (SL) on graphene consisting of very high and thin (δ-function) barriers. The energy spectrum was obtained analytically and I studied the transmission through a finite number of barriers.

- **Chapter 8**: In the next step I considered a combination of one-dimensional (1D) magnetic and potential superlattices (SL) on graphene with zero average potential and magnetic field. The energy spectrum, electron collimation and the conditions to open a gap are studied.

- **Chapter 9**: Circular symmetric inhomogeneous magnetic field profiles of the magnetic field as magnetic dots are considered. I study the existence of quasi bound states using the local density of states technique. The properties of electrons with parabolic dispersion in such circular inhomogeneous magnetic fields are compared with those of Dirac electrons with a linear dispersion.
1.4. MOTIVATION AND OUTLINE

- **Chapter 10**: The study of chapter 9 is extended to the scattering states of an electron in graphene-based single magnetic dots and magnetic rings and combinations of both.

- **Chapter 11**: The electrical transport of two-dimensional (2D) massless Dirac electrons in the presence of a random array of circular mass barriers is calculated. The inverse momentum relaxation time and the Hall factor are calculated and used to obtain the magneto- and Hall resistivity components within linear transport theory.

- **Chapter 12**: The study of previous chapter is generalized to the case of scattering on a random array of circular magnetic flux tubes.
2

Electronic properties of graphene

2.1 Tight binding model

The tight binding model is an approach used to calculate the electronic band structure using an approximate set of wave functions based upon a superposition of wave functions for isolated atoms located at each atomic site. The method is closely related to the linear combination of atomic orbitals (LCAO) method. Graphene is composed of carbon atoms arranged in a hexagonal lattice with each carbon atom covalently bonded to three other carbon atoms. Core electron orbitals do not overlap much with the orbitals of adjacent atoms, which result in electrons localized at the atomic positions. Due to this localization, the electrons are considered as tight-bonded to the atoms. The tight binding model describes the band structures by only a few parameters, whose values are chosen such that it reproduces the experimental results or the outcome of first-principles calculations.

We consider the electrons to be localized in each atomic position. The probability to find an electron on an adjacent atom is small and therefore we can expand the Bloch wave function of the crystal by a linear combination of local Wannier functions,

\[ \psi_{n,k}(r) = \frac{1}{\sqrt{N}} \sum_{R} \Phi_{n}(R,r)e^{i\mathbf{k} \cdot r}, \]  

(2.1)

where \( \mathbf{R} \) is the real-space lattice vectors of \( C \) atoms. The functions \( \Phi_{n}(R,r) \) are called Wannier functions and \( N \) is the number of unit cells in the crystal. To develop a useful model several approximations must be made. The first approximation is the so-called two-center approximation, in which the Hamiltonian is approximated by the atomic Hamiltonian centered on the atomic positions in the unit cell \( \mathbf{R} \). The Wannier functions are approximated by the eigenfunctions of the atomic Hamiltonian, with the atomic orbitals \( \phi_{\mu,n}(\mathbf{r} - \mathbf{t}_l - \mathbf{R}) \), where \( \mathbf{t}_l \) is the position vector of the atom \( l \) inside the primitive unit cell at \( \mathbf{R} \) and \( s \) is the spin.
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state of the $\mu^{th}$ orbital. The resulting on-site Bloch wave function is,

$$\psi_{k,n}(r) = \frac{1}{\sqrt{N}} \sum_R \phi_{\mu,s}(r - t_\ell - R)e^{i\mathbf{k}\cdot\mathbf{r}},$$  \hfill (2.2)

which obey the Bloch theorem:

$$\Psi_{k,j}(r + \mathbf{R}') = \exp(i\mathbf{k} \cdot \mathbf{R}')\Psi_{k,j}(r).$$  \hfill (2.3)

In order to find the Hamiltonian matrix element we start with the Schrödinger equation,

$$H\Psi_k(r) = E_k\Psi_k(r).$$  \hfill (2.4)

The crystal wave function $\Psi_k(r)$ can be expanded in the basis of the on-site Bloch wave functions,

$$\Psi_k(r) = \sum_i c_{k,i}\psi_{k,i}(r).$$  \hfill (2.5)

Substituting Eq. (2.5) in Eq. (2.4) and using the orthogonality of the Bloch wave functions we obtain,

$$\sum_{i,j} c_{k,j}^* c_{k,i} \left[ \Psi_{k,j}(r) H\psi_{k,i}(r) - E_k\Psi_{k,j}(r)\psi_{k,i}(r) \right] = 0.$$  \hfill (2.6)

The Hamiltonian matrix element can be defined as,

$$H_{i,j}(k) = \frac{1}{N} \sum_{R,R'} e^{i\mathbf{k} \cdot (#R-R')} \int dr \phi_j^*(r-\mathbf{R})H\phi_i(r-\mathbf{R}),$$  \hfill (2.7)

and the overlap matrix elements are defined as,

$$S_{i,j}(k) = \frac{1}{N} \sum_{\mathbf{R},\mathbf{R}'} e^{i\mathbf{k} \cdot (#R-R')} \int dr \phi_j^*(r-\mathbf{R})\phi_i(r-\mathbf{R}).$$  \hfill (2.8)

Due to the fact that the atomic orbitals centered at the different sites are not orthogonal, the overlapping integral in general has a non-zero but small value. This non-orthogonality is useful to obtain the electronic spectrum over a wide range of wave vector space. Substituting Eqs. (2.6) and (2.7) in Eq. (2.8), we find the energy spectrum for fixed $k$ as

$$E_k = \sum_{i,j} H_{i,j}(k)c_{k,j}^*c_{k,i}/\sum_{i,j} S_{i,j}(k)c_{k,j}^*c_{k,i}.$$  \hfill (2.9)

Minimizing the energy using $\partial E_k/\partial c_{k,i}^* = 0$, we obtain the secular equation as,

$$\sum_i \left[ H_{i,j}(k) - E_kS_{i,j}(k) \right] c_{k,i} = 0.$$  \hfill (2.10)
2.1. TIGHT BINDING MODEL

2.1.1 Tight binding model for monolayer graphene

We consider a monolayer graphene as shown in Fig. 2.1 with unit cell that contains two atoms denoted by $A$ and $B$. The positions of type $A$ atoms can be generated using linear combination of basis vectors,

$$A(n_1, n_2) = n_1 a_1 + n_2 a_2,$$  \hspace{1cm} (2.11)

with lattice vectors $a_1$ and $a_2$ given by,

$$a_1 = \left( \frac{3}{2}, \frac{\sqrt{3}}{2} \right) a, \quad a_2 = \left( \frac{3}{2}, -\frac{\sqrt{3}}{2} \right) a \hspace{1cm} (2.12)$$

where $a = 0.142$ nm, is the carbon-carbon atom distance and $n_1, n_2$ are two arbitrary integer number. The $A$ sublattices are connected to $B$ sublattices using the three sublattice vectors

$$\delta_1 = \left( \frac{1}{2}, \frac{\sqrt{3}}{2} \right) a, \quad \delta_2 = \left( \frac{1}{2}, -\frac{\sqrt{3}}{2} \right) a, \quad \delta_3 = \left( -1, 0 \right) a.$$  \hspace{1cm} (2.13)

The position of $B$ sublattices are given by $B(m_1, m_2) = m_1 a_1 + m_2 a_2 + \delta_1$, where $m_1$ and $m_2$ are two integer numbers. The six second nearest neighbors are given by,

$$\delta' = \{ a_1, a_2, a_1 - a_2, a_2 - a_1, -a_1, -a_2 \}.$$  \hspace{1cm} (2.14)
CHAPTER 2. ELECTRONIC PROPERTIES OF GRAPHENE

The reciprocal lattice of graphene is also a two dimensional triangular lattice with reciprocal lattice vectors given by

$$b_1 = \frac{2\pi}{3a} \left( 1 \quad 1/\sqrt{3} \right), \quad b_2 = \frac{2\pi}{3a} \left( 1 \quad -1/\sqrt{3} \right),$$

(2.15)

and the hexagonal Brillouin zone shown in Fig. 2.1(b) and two different corners of the Brillouin zone are defined by the wave vectors

$$K = \frac{2\pi}{3a} \left( 1 \quad 0 \right), \quad K' = \frac{2\pi}{3a} \left( -1 \quad 0 \right).$$

(2.16)

These points are inequivalent because they cannot be connected by the reciprocal lattice vectors Eq. (2.15). The degeneracy of the high-symmetry $K$ and $K'$ points called valley degeneracy, is a consequence of the time inversion symmetry. We can reach to the remaining $K$ and $K'$ points through a rotation by an angle $\pm 2\pi/3$.

There are two atoms per unit cell in the graphene lattice which forms two triangular sublattices $A$ and $B$ and the Bloch wave functions can be build up by linear combination of the two sublattice Bloch wave functions,

$$\Psi_k(r) = a_k \Psi_k^A(r) + b_k \Psi_k^B(r)$$

(2.17)

where the $a_k$ and $b_k$ are complex functions of the quasi-momentum $k$ and can be understood as the amplitude of the sublattice pseudospin. As we shown in Fig. 2.2, the pseudospin up state equate to the electron density localized at sublattice $A$ and the pseudospin down state at sublattice $B$. With taking the nearest neighbor approximation (NNA) into account the hopping amplitude is given by

$$H^{AB}(k) = \frac{1}{N} \sum_{R, R'} e^{i \mathbf{k} \cdot (\mathbf{R} - \mathbf{R}')} \int d^2 r \phi^*_A,\sigma(r - \mathbf{R}') H \phi_B,\sigma'(r - \mathbf{R})$$

$$= \sum_{R''} e^{i \mathbf{k} \cdot \mathbf{R}''} \int d^2 r \phi^*_A,\sigma(r) H \phi_B,\sigma'(r - \mathbf{R}' - \mathbf{b}_1)$$

$$\approx e^{-i \mathbf{k} \cdot \mathbf{b}_1} \sum_{m=1}^{3} e^{i \mathbf{k} \cdot \mathbf{b}_m} \int d^2 r \phi^*_A(r) H \phi_B(r - \mathbf{b}_m)$$

(2.18)

$$= e^{-i \mathbf{k} \cdot \mathbf{b}_1} \sum_{m=1}^{3} t_m e^{i \mathbf{k} \cdot \mathbf{b}_m}$$

$$= (H^{BA}(k))^*.$$
where \( \sigma \) correspond to the different atomic orbitals. The overlap parameters between orbitals on NN sites are given by,

\[
S_{AB}(k) \approx e^{-i k \cdot \delta_1} \sum_{m=1}^{3} e^{i k \cdot \delta_m} \int d^2 r \phi_{A,\sigma}^*(r) \phi_{A,\sigma'}(r - \delta_m)
\]

\[
= e^{-i k \cdot \delta_1} \sum_{m=1}^{3} s_m e^{i k \cdot \delta_m}
\]

\[
= (S_{BA}(k))^*,
\]

(2.19)

and the on-site overlap is given by,

\[
S_{AA}(k) = S_{BB}(k) \approx \int d^2 r \phi_{\sigma}^*(r) \phi_{\sigma}(r) = \delta_{\sigma \sigma'}.
\]

(2.20)

We also consider the next nearest neighbor (NNN) hopping which connects the same sublattice sites,

\[
H_{AA}(k) = H_{BB}(k) = \frac{1}{N} \sum_{R,R'} e^{i k \cdot (R-R')} \int d^2 r \phi_{A,\sigma}^*(r - R') H \phi_{A,\sigma'}(r - R)
\]

\[
= \sum_{R''} e^{i k \cdot R''} \int d^2 r \phi_{\sigma}^*(r) H \phi_{\sigma'}(r - R'' - b_1)
\]

\[
\approx 6 \sum_{i=1}^{3} e^{i k \cdot a_i} \int d^2 r \phi_{\sigma}^*(r) H \phi_{\sigma'}(r - b_m)
\]

\[
= 2 t' \sum_{i=1}^{3} \cos k \cdot a_i
\]

\[
= \varepsilon_{\tau} \delta_{\sigma \sigma'}
\]

(2.21)

where \( \varepsilon_{\tau} \) correspond to the energy of the atomic orbital \( \tau = s, p, d, \ldots \) and \( t' \) is the NNN hopping parameter. For the electronic properties of graphene we use the particular case where only the \( \pi \) bonding created by the transverse \( p_z \) orbitals from the \( sp^2 \) hybridization of carbon atom are considered. Using this assumption, the off diagonal elements of the hopping matrix is given by

\[
H_{AB}^{pz,pz} = (H_{BA}^{pz,pz})^* = \omega_k,
\]

(2.22)

and the on-site hopping matrix elements for NNN are

\[
H_{AA}^{pz,pz} = (H_{BB}^{pz,pz})^* = \varepsilon_{pz},
\]

(2.23)
and the overlap elements are
\[
S_{p_z,p_z}^{AB} = (S_{p_z,p_z}^{AB})^* = s\omega_k, \quad (2.24)
\]
\[
S_{p_z,p_z}^{AA} = (S_{p_z,p_z}^{BB})^* = 1.
\]
The phase function \(\omega_k\) is a sum over the NN phase factors,
\[
\omega_k = \sum_i e^{ik\cdot\delta_i} \quad (2.25)
\]
substituting the matrix elements in Eq. (2.10) we obtain the secular equation,
\[
\det \begin{bmatrix} \varepsilon_{p_z} - \varepsilon_k & (t - s\varepsilon_k)\omega_k \\ (t - s\varepsilon_k)\omega_k^* & \varepsilon_{p_z} - \varepsilon_k \end{bmatrix} = 0, \quad (2.26)
\]
where the two solutions of this equation correspond to the valence (\(\alpha = +1\)) and the conductance band (\(\alpha = -1\)), and are given by,
\[
\varepsilon_k = \frac{\varepsilon_{p_z} + \alpha t|\omega(k)|}{1 + \alpha s|\omega(k)|}, \quad (2.27)
\]
where
\[
|\omega(k)| = \sqrt{3 + 2\sum_{i\neq j}\cos k \cdot (\delta_i - \delta_j)} = \sqrt{3 + f(k)}. \quad (2.28)
\]
2.1. TIGHT BINDING MODEL

Figure 2.3: (a) Graphene band structure and linear spectrum close to Dirac point. (b) 2D Brillouin zone.

and then

\[ f(k) = 2 \cos (\sqrt{3} k_y a_0) + 4 \cos (\sqrt{3} k_y a_0 / 2) \cos (3 k_x a_0 / 2). \]  

Expanding the Eq. (2.27) using the fact that \( s \ll 1 \) and \( \varepsilon_{p_z} \ll t \), we obtain,

\[
\varepsilon_k \approx (\varepsilon_{p_z} + \alpha t |\omega(k)|)(1 - \alpha s |\omega(k)|)
= \varepsilon_{p_z} + \alpha t |\omega(k)| - st|\omega(k)|^2 \\
= \alpha t \sqrt{3 + f(k)} + t'f(k), \]

where we have \( f(k) = |\omega(k)|^2 - 3 \) and \( t' = t_2 - st \). The parameters \( t \) and \( t' \) where estimated using first-principle calculations yielding the value \( t \approx -3eV \) for NN hoping and \( 0.02t \leq t' \leq 0.2t \) for the NNN hopping parameter. The conduction
Figure 2.4: Schematic representation of the helicity in the two valleys including the momentum and pseudo spin direction.

\( \alpha = -1 \) and valence \( \alpha = +1 \) bands in the energy dispersion (see Fig. 2.3) are connected by the positions of the Dirac points \( K(K') \) given by the roots of the energy dispersion \( \varepsilon_k = 0 \). The valence band is completely filled and the conduction band is completely empty due to the fact that only one electron (with spin-up or spin-down) of each carbon atom contributes to the \( \pi \) band. When \( t' = 0 \) then the energy dispersion has electron-hole symmetry \( \varepsilon_k^\alpha = -\varepsilon_k^{-\alpha} \). Hamiltonian has time reversal symmetry \( H_k = H^*_k \) and it means that \( \varepsilon_k = \varepsilon_{-k} \) and a pair of Dirac points occurs with doubly degenerate zero-energy state. This is the so called valley degeneracy which can survive for small energy. The positions of these Dirac points are given by Eq. (2.16).

### 2.1.2 Effective Hamiltonian and continuum limit

We can define an effective Hamiltonian as

\[
H = \begin{bmatrix}
t' & t \omega^*(k) \\
t \omega(k) & t'
\end{bmatrix},
\]  
(2.31)

and the eigenstate of this Hamiltonian is given by

\[
\Psi_k = \begin{pmatrix}
a_k^\alpha \\
b_k^\alpha
\end{pmatrix}
\]  
(2.32)
2.1. Tight Binding Model

neglecting the NNN hoping parameter $t'$ we obtain the eigenvalues given by

$$\lambda = \alpha \frac{\omega^*(\mathbf{k})}{|\omega(\mathbf{k})|},$$  \hspace{1cm} (2.33)

and thus the eigenstates are

$$\Psi_k = \frac{e^{i\mathbf{k} \cdot \mathbf{r}}}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{-i\varphi} \end{pmatrix},$$  \hspace{1cm} (2.34)

with $\varphi = \arctan \left( \frac{\text{Im}(\omega(\mathbf{k}))}{\text{Re}(\omega(\mathbf{k}))} \right)$.

Continuum Limit

Expanding the energy dispersion Eq. (2.30) close to the $K(K')$ point using $k = K + \kappa$ with $|\kappa| \ll |K|$ we find to first order [35],

$$\varepsilon^\alpha_{k,\eta = \pm} = \alpha v_F |\kappa| + O[(\kappa/K)^2]$$ \hspace{1cm} (2.35)

with $v_F = 3t a_0/2\hbar$. In Eq. (2.35) $\varepsilon_k$ to first approximation is independent from the valley pseudospin $\eta$. This results in an effective Hamiltonian that is valid close to the Dirac points,

$$H = \eta \hbar v_F (k_x \sigma_x + \eta k_y \sigma_y),$$  \hspace{1cm} (2.36)

where $\sigma_i$ are the Pauli matrices and $\eta = \pm$ corresponds to the two individual $K(+) \text{ and } K'(-)$ points. This Hamiltonian is simply the 2D massless Dirac-Weyl Hamiltonian with $c \rightarrow v_F$. It is useful to use the four-spinor representation with the effective low-energy Hamiltonian as

$$H_q = \hbar v_F \mathbf{\tau} \otimes \mathbf{q} \cdot \mathbf{\sigma},$$  \hspace{1cm} (2.37)

where

$$\mathbf{\tau} \otimes \mathbf{\sigma} = \begin{pmatrix} \mathbf{\sigma} & 0 \\ 0 & -\mathbf{\sigma} \end{pmatrix}. \hspace{1cm} (2.38)$$

The eigenstates are given by

$$\Psi_{q,\alpha}^{\eta = \pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \alpha e^{i\phi} \\ 0 \\ 0 \end{pmatrix} \quad \Psi_{q,\alpha}^{\eta = -} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \\ -\alpha e^{i\phi} \end{pmatrix}$$ \hspace{1cm} (2.39)

where $\phi = \arctan(q_y/q_x)$. The Pauli matrices in Eq. (2.37) are representing the sublattice pseudospin with spin up for one of the sublattices $A \text{ or } B$ and spin down
for the other one. The valley isospin is described by the second set of Pauli matrices \( \tau^z \) in the Hamiltonian of Eq. \((2.37)\). The twofold valley degeneracy is indirectly related to the two different sublattices. The expansion of the spectrum around the Dirac point including \( t' \) up to second order in \( q/K \) is given by

\[
E_{\pm}(q) \approx 3t' \pm v_F |q| - \left( \frac{9t' a^2}{4} \pm \frac{3ta^2}{8} \sin(3\theta_q) \right) |q|^2.
\] (2.40)

In the presence of \( t' \) the position of the Dirac point shifts and it breaks the electron-hole symmetry. Note that up to order \( (q/K)^2 \) the dispersion depends on the direction in momentum space and has a threefold symmetry. This is the so-called trigonal warping of the electronic spectrum (see Fig. 2.3 (b)).

### 2.1.3 Helicity and Chirality

Mathematically a figure has chirality if it can not be mapped to its mirror image by only rotations and translations. Helix and Möbius are two famous 2D chiral objects in three-dimensional space. Many other familiar objects which exhibit the chiral symmetry are the human body, gloves, and shoes. In particle physics chirality is determined by whether the particle transforms in a right or left handed representation of the Poincaré group. Helicity is the projection of the spin of the particle onto the direction of its motion.

In graphene we can write the helicity operator for the sublattice pseudo spin as,

\[
h_q = \sigma \cdot \frac{q}{|q|}.
\] (2.41)

As shown in Fig. 2.4 the helicity of the electron is right-handed if the pseudospin and momentum are in the same direction and left-handed if the pseudo spin and momentum are in opposite direction. For massless particles chirality is the same as helicity. Electrons in graphene due to the linear spectrum close to the Dirac points have well defined chirality. The helicity operator commutes with the Hamiltonian and it has the same eigenstates with eigenvalues, \( h = \pm 1 \),

\[
h_q \Psi_K = \pm \Psi_K,
\]

\[
h_q \Psi_{K'} = \mp \Psi_{K'}.
\] (2.42)

It is also possible to present the Hamiltonian using the helicity operator,

\[
H = \eta h v_f q |h_q|,
\] (2.43)

where is the valley degeneracy. The band index \( \alpha = \pm 1 \) can be determined using \( \alpha = \eta h \). The helicity eigenvalue is a good quantum number for energy close to the \( K \) and \( K' \) points.
2.1.4 Klein tunneling

In the presence of a slowly varying potential, chirality for an elastic scattering process remains a good quantum number since such a potential can not mix the $K$ and $K'$ valleys. When intervalley scattering and the lack of symmetry between sublattices are neglected for a normal incident electron a potential barrier shows no reflection and the electron is fully transmitted. This effect is known as Klein tunneling or Klein paradox [31].

In order to present this problem in more detail we start with the low-energy Dirac Hamiltonian given by Eq. (2.36). For low energy we can neglect intervalley scattering and the electrons in $K$ and $K'$ behave independently. Then we can write the equation $H \Psi(x, y) = E \Psi(x, y)$, which admits spinor solutions of the form

$$\Psi(x, y) = \begin{pmatrix} \psi_I(x, y) \\ \psi_{II}(x, y) \end{pmatrix}.$$  (2.44)

We will consider two systems: (a) potential step and (b) potential barrier, along $x$ direction. Due to the translational invariance along the $y$-direction we attempt solutions of the form $\Psi(x, y) = \exp(ik_y y) (\phi_1(x), \phi_2(x))^T$ with $T$ denoting the transpose of the row vector. Then $\phi_1(x)$ and $\phi_2(x)$ obey the coupled first-order differential equations

$$-i\hbar v_F \left[ \frac{d}{dx} + k_y \right] \phi_2 = \varepsilon \phi_1, \quad (2.45a)$$
$$-i\hbar v_F \left[ \frac{d}{dx} - k_y \right] \phi_1 = \varepsilon \phi_2, \quad (2.45b)$$

where $\varepsilon = E - V$. For a step potential $V(x) = V \Theta(x)$ (see Fig. 2.5(a)) the solutions of this coupled set of differential equations in dimensionless units are

$$\Psi_1(x, y) = e^{ik_y y} \begin{pmatrix} e^{ik_1 x} + re^{-ik_1 x} \\ s_i \left[ e^{ik_1 x+i\theta} - re^{-ik_1 x-i\theta} \right] \end{pmatrix}.$$  (2.46)
\[ \Psi_2(x, y) = e^{ik_y y} \left( t e^{\pm ik_x x} \pm s_i t e^{\pm (ik_x x + i\varphi)} \right) \] (2.47)

where \( s_i = \text{sgn}(E - V_i) \), \( k_i = \sqrt{\varepsilon_i^2 - k_y^2} \), with \( i = 1, 2 \), \( \tan \theta = k_y/k_1 \) and \( \tan \varphi = k_y/k_2 \). Matching the waves at \( x = 0 \), we obtain the transmission probability \( T = tt^* \) and consider two different cases: 1) \( E < V \),

\[ t_{E<V} = \frac{2 \cos \theta}{e^{-i\theta} + e^{-i\varphi}}; \quad T_{E<V} = \frac{2 \cos^2 \theta}{1 + \cos(\theta - \varphi)}, \] (2.48)

and 2) \( E > V \)

\[ t_{E>V} = \frac{2 \cos \theta}{e^{-i\theta} + e^{i\varphi}}; \quad T_{E>V} = \frac{2 \cos^2 \theta}{1 + \cos(\theta + \varphi)}. \] (2.49)

Using the fact that the momentum of the electron in the \( y \) direction is continuous at \( x = 0 \), we obtain Snell’s law as \( \sin \theta = \frac{1 - V}{E} \sin \varphi \). When \( E < V \) or \( E - V < 0 \) the step potential acts like a medium with negative refraction index (see Fig. 2.5(b)) and an incident beam of electrons can be focused in the potential step [36]. The critical angle is \( \sin \theta_c = \frac{1 - V}{E} \). For \( E < V/2 \) we have that \( \theta_c \) is imaginary (\( k_1 \) is imaginary) and thus the electron is localized.

Next we consider a potential barrier with width \( W \) as shown in Fig. 2.6. From
the point of view of optics it is like a medium with refraction index $1 - \frac{V}{E}$. When we inject a wave with incident angle $\theta$, it splits into transmitted and reflected waves. The transmitted wave inside the barrier will resonate between the two edges at $x = 0$ and $W$ as shown in Fig. 2.7. Analogous with optical waves the difference in the optical paths along the barrier is,

$$\Delta L = \left(1 - \frac{V}{E}\right)(BC + CD) - (BN),$$

(2.50)

where $BC = CD = \frac{W}{\cos \varphi}$, and $BN = 2W \tan \varphi \sin \theta$. Using $\sin \theta = (1 - V/E) \sin \varphi$, we obtain

$$\Delta L = 2\left(1 - \frac{V}{E}\right)W \cos \varphi.$$  \hspace{1cm} (2.51)

The total transmission is given by

$$T = |t_1|^2 + |t_2|^2 + 2|t_1||t_2| \cos \delta,$$

with the corresponding phase difference,

$$\delta = k_1 \Delta L = 2k_1 \left(1 - \frac{V}{E}\right)W \cos \varphi.$$ \hspace{1cm} (2.52)

The transmission is maximum when $|\delta| = 0, 2\pi, 4\pi, \ldots$, and minimum when $|\delta| = \pi, 3\pi, \ldots$.

In order to obtain the total transmission we introduce $r$ and $t$ to be the reflection and transmission coefficient for the potential step outside the barrier, and $r'$ and $t'$ the corresponding coefficients for inside the barrier. The different combinations of transmitted waves through the barrier are,

$$tt', \ r't'^2 e^{i\delta}, \ldots , t't'^{2(n-1)} e^{i(n-1)\delta}, \ldots$$ \hspace{1cm} (2.53)
and we obtain the total transmission amplitude by summing over all terms,

\[ t_{tot} = t t' \left( 1 + r' e^{i \delta} + \ldots + r'^{2(n-1)} e^{i(n-1) \delta} + \ldots \right) = \frac{t t'}{1 - r' e^{i \delta}}, \]

(2.54)

and the corresponding transmission probability \( T_{tot} = t_{tot} t_{tot}^* \) is,

\[ T_{tot} = \frac{1}{1 + F \sin^2 \left( \frac{\delta}{2} \right)}, \]

(2.55)

where \( F = 4R/(1 - R)^2 \) with \( R = |r'|^2 \) and \( T = t t' \). Using Eqs. (2.46) and (2.47) we obtain \( r' \) and thus,

\[ F = \frac{[1 - \cos(\theta - \varphi)][1 + \cos(\theta + \varphi)]}{\cos^2 \theta \cos^2 \varphi}, \]

(2.56)

where \( F \) is the coefficient of finesse. Substituting Eq. (2.56) in (2.55) we find the known transmission probability for a single barrier [32],

\[ T = \frac{\cos^2 \theta \cos^2 \varphi}{[\cos(k_2 W) \cos \theta \cos \varphi]^2 + \sin^2(k_2 W)(1 - \sin \theta \sin \varphi)^2}, \]

(2.57)

with \( \delta = 2k_2 W \). Substituting \( k_2 W = n\pi \) in Eq. (10) we obtain the energies \( E \) at which the resonances occur (i.e., \( T = 1 \))

\[ E = V \pm \left[ k_2^2 + n^2 \pi^2/W^2 \right]^{1/2}. \]

(2.58)

For normal incident wave with \( \theta = 0 \) we find \( T = 1 \) as expected from the Klein paradox. Note that \( T(\theta) = T(-\theta) \), and for values of \( k_2 W \) satisfying the relation \( k_2 W = n\pi \), with \( n \) an integer, the barrier becomes completely transparent since \( T = 1 \), independent of the value of \( \theta \).

### 2.1.5 High mobility and minimum conductivity

Transport measurements in graphene show remarkably high electron mobility at room temperature [2]. The nearly symmetric conductance measured experimentally show that mobilities for holes and electrons should be nearly the same [2], and it is almost independent of temperature [11, 12], which implies that the dominant scattering mechanism is defect scattering.

In spite of vanishing carrier density near the Dirac points, graphene shows a minimum conductivity close to the conductivity quantum \( 4e^2/h \) per carrier type
2.1. TIGHT BINDING MODEL

[11]. There is a number of theories [37–42] to describe the minimum conductivity but still the origin of this minimum conductivity is unclear. Most theories suggest that the minimum conductivity should be $4e^2/\pi \hbar$, which in comparison with experimental measurement is $\pi$ times smaller [2] and depends on impurity concentration [43]. This disagreement is well known as "the mystery of missing a $\pi$" [2]. Close to the Dirac point, graphene conducts as randomly distributed electron and hole puddles due to graphene inhomogeneity from graphene ripples and defects. Theory did not take into account these inhomogeneity, and possibly this can explain the higher conductivity in the experimental data (see Fig. 2.8).

Figure 2.8: (a) Ambipolar electric field effect in single-layer graphene. The insets show its conical low-energy spectrum. (b) Minimum conductivity of graphene. Independent of their carrier mobility. (Figures are from [2])

2.1.6 Bilayer graphene

As with monolayer graphene, bilayer graphene consists of two graphene layers on top of each other. A bilayer graphene has a zero bandgap and thus behaves like a metal. But a bandgap can be introduced between the conduction and valence band. The bilayer structure, in $AB$ stacking configuration is shown in Fig. 2.9. The tight binding Hamiltonian for bilayer graphene can be written as [35, 44],

$$
H = -\gamma_0 \sum_{i,j} (a_{m,i,s}^\dagger b_{m,i,s} + H.c.) - \gamma_1 \sum_{j,s} (a_{1,j,s}^\dagger a_{2,j,s} + H.c.) \\
- \gamma_2 \sum_{j,s} (a_{1,j,s}^\dagger b_{2,j,s} + a_{2,j,s}^\dagger b_{1,j,s} + H.c.) - \gamma_3 \sum_{j,s} (a_{1,j,s}^\dagger b_{2,j,s} + H.c.),
$$

(2.59)
where $a_{m,i,s}(b_{i,m,s})$ is the annihilation of an electron with spin $s$ at site $R_i$ of sublattice $A(B)$. Different hopping parameters are $\gamma_i$ approximately given by $\gamma_0 = t$, $\gamma_1 \approx 0.4$ eV, $\gamma_3 \approx 0.3$ eV and $\gamma_4 = 0.04$ eV in graphite. Neglecting the $\gamma_4$ we can write the Hamiltonian close to the $K$ and $K'$ valleys as

$$H = \begin{pmatrix}
-\Delta/2 & v_3 \pi & 0 & v\pi \\
v_3\pi^\dagger & \Delta/2 & v\pi & 0 \\
0 & v\pi^\dagger & \Delta/2 & \xi \gamma_1 \\
v\pi & 0 & \xi \gamma_1 & -\Delta/2
\end{pmatrix}$$

(2.60)

where $v = (\sqrt{3}/2)a\gamma_0/h$ is the in-plane velocity, $v_3 = (\sqrt{3}/2)a\gamma_3/h$ is an effective velocity where $v_3 \ll v$ velocity, $\pi = p_x + ip_y$, $\pi^\dagger = p_x - ip_y$, $P = (p_x,p_y) = p(\cos \phi, \sin \phi)$ is the momentum and $\xi = \pm 1$ for two different valleys $K$ and $K'$, $\Delta = \epsilon_2 - \epsilon_1$ is the difference between on-site energies in the two layers. Corresponding eigenstates are,

$$\Psi_K = \begin{pmatrix}
\psi_{A1} \\
\psi_{B2} \\
\psi_{A2} \\
\psi_{B1}
\end{pmatrix}, \quad \Psi_{K'} = \begin{pmatrix}
\psi_{B1} \\
\psi_{A1} \\
\psi_{B2} \\
\psi_{A2}
\end{pmatrix}$$

(2.61)

From the Hamiltonian in Eq. (2.60), one obtains the energy band as,

$$\epsilon_{\pm,\alpha}^2 = \frac{\gamma_1^2}{2} + \frac{\Delta^2}{4} + \left(v^2 + \frac{v_3^2}{2}\right)p^2 + (-1)^\alpha \sqrt{\Gamma}$$

(2.62)

$$\Gamma = \frac{1}{4}(\gamma_1^2 - v_3^2p^2)^2 + v^2p^2[\gamma_1^2 + \Delta^2 + v_3^2p^2] + 2\xi \gamma_1 v_3 v^2p^3 \cos 3\phi.$$  

(2.63)

In the absence of layer asymmetry these bands are plotted in Fig. 2.10 (a). The dispersion $\epsilon_{\pm,1}$ are those that touch at the K point. In the presence of finite valley
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Figure 2.10: Electronic band of bilayer graphene for (a) $\Delta = 0$ and (b) $\Delta \neq 0$.

asymmetry $\Delta$ as shown in Fig. 2.10 (b) a gap will open between the upper band $\epsilon_{+,1}$ and the lower one $\epsilon_{-,1}$.

In order to study the transport properties of bilayer graphene it is useful to find an effective low-energy Hamiltonian. Such effective Hamiltonian can be obtained by considering $\gamma_1$ large in comparison with $\gamma_3$ and $\gamma_4$. Using this approximation we obtain a two component Hamiltonian describing the effective hopping between two site $A_1$ and $B_2$ as,

$$ H = \frac{1}{2m} \begin{pmatrix} 0 & \pi \cr \pi & 0 \end{pmatrix} + \xi \gamma_3 \begin{pmatrix} 0 & \pi \cr \pi & 0 \end{pmatrix} - \xi \Delta \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \frac{\psi^2}{\gamma_1} \begin{pmatrix} \pi \pi \cr \pi & \pi \end{pmatrix}, \quad (2.64) $$

where $m = \gamma_1/2v^2$. This Hamiltonian is applicable when $\epsilon < \gamma_1/4$. The eigenstates for two different valleys $K$ and $K'$ are given by,

$$ \Psi^K_{\xi=+1} = \begin{pmatrix} \psi_{A_1} \\ \psi_{B_2} \end{pmatrix}, \quad \Psi^{K'}_{\xi=-1} = \begin{pmatrix} \psi_{B_1} \\ \psi_{A_1} \end{pmatrix}. \quad (2.65) $$

Note that the components are reversed for different valleys.

2.2 In the presence of magnetic field

2.2.1 Homogenous magnetic field

An electron in a single graphene layer, in the presence of a perpendicular magnetic field $B(x)$, that may vary along the $x$ direction is described by the Hamiltonian,

$$ H = v_f \tau_z \otimes \mathbf{\sigma} \cdot \mathbf{\Pi}, \quad (2.66) $$
here we replaced the momentum by its gauge-invariant form \[45\] also called the minimal substitution,

\[ p \rightarrow \Pi = p + eA(r) \]

(2.67)

where \( p \) is the momentum operator, and \( A(x) \) the vector potential that generates the magnetic field \( B = \nabla \times A \). Not the \( p \) nor the \( A \) are gauge invariant. Adding a gradient of an arbitrary function \( \nabla f \) to the vector potential \( A \) result in the same magnetic field. Under a gauge transformation one needs to transform \( p \rightarrow p - e\nabla f \) in order to have a gauge invariant \( \Pi \). In the context of electrons on a lattice, transformation in Eq. (2.67) is valid as long as the lattice spacing \( a \) is much smaller than the magnetic length \( \ell_B \),

\[ \ell_B = \sqrt{\frac{eB}{\hbar}}, \]

(2.68)

The lattice spacing \( a \) is in the order of 0.142 nm and then \( a \ll \ell_B \) is satisfied for the high-magnetic fields achieved in labs of around 80T. We consider such Dirac electron in the presence of a homogeneous magnetic field \( B_0 \). Let us work in the Landau gauge, where \( A(x) = (0, Bx, 0) \). We can write Eq. (2.66) explicitly as

\[ H = -iv_Fh \begin{pmatrix} 0 & \partial_x - i\partial_y - eBx/\hbar \\ \partial_x + i\partial_y - eBx/\hbar & 0 \end{pmatrix}. \]

(2.69)

Then the equation \( H\Psi(x,y) = E\Psi(x,y) \) admits solutions

\[ \Psi(x,y) = \begin{pmatrix} \psi_A(x,y) \\ \psi_B(x,y) \end{pmatrix}, \]

(2.70)

with \( \psi_A(x,y), \psi_B(x,y) \) obeying the coupled equations

\[ i \left[ \frac{\partial}{\partial x} - i\frac{\partial}{\partial y} + \frac{eB}{\hbar} x \right] \psi_B + E\psi_A = 0, \]  

(2.71a)

\[ i \left[ \frac{\partial}{\partial x} + i\frac{\partial}{\partial y} - \frac{eB}{\hbar} x \right] \psi_A + E\psi_B = 0. \]  

(2.71b)

For such a gauge, \( [H, p_y] = 0 \), and \( p_y \) is a good quantum number and due to the translational invariance along the \( y \) direction we assume solutions of the form \( \Psi(x,y) = \exp(ik_yy)(a(x), b(x))^T \), \( T \) denoting the transpose of the row vector. Then Eqs. (5.37a) and (5.37b) take the form

\[ -i\hbar v_F \left[ \frac{d}{dx} + (k_y + x/\ell_B) \right] b = Ea, \]  

(2.72a)

\[ -i\hbar v_F \left[ \frac{d}{dx} - (k_y + x/\ell_B) \right] a = Eb. \]  

(2.72b)
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Operating on Eqs. (2.72) with \(-i(d/dx - (k_y + x))\) gives

\[
\left[ \frac{d^2}{dx^2} - (k_y + x)^2 + 1 + \left( \frac{\ell_B^2}{\hbar^2 v_F^2} \right) E^2 \right] c_\pm = 0, \tag{2.73}
\]

where \(c_- = a\) and \(c_+ = b\). The solution of Eq. (2.73) are the well-known Hermite polynomials \(H(x)\). For \(c_- = a\) the wave function is \(a(x) = \exp(-z^2/4) H_{E^{2}/2-1}(x+k_y)\) and the energy spectrum

\[
E_n = \pm \frac{\hbar v_F}{\ell_B} \sqrt{2n+1}. \tag{2.74}
\]

Thus, we have the standard expression for Landau levels for Dirac electron with lowest level

\[
E_0 = \sqrt{2} \frac{\hbar v_F}{\ell_B}. \tag{2.75}
\]

Repeating this procedure for \(c_+ = b\) gives \(b(x) = \exp(-z^2/4) H_{E^{2}/2}(x+k_y)\) with spectrum

\[
E_n = \pm \frac{\hbar v_F}{\ell_B} \sqrt{2n} \propto \sqrt{nB}. \tag{2.76}
\]

Notice the difference of these spectra from the one for the Schrödinger electrons with \(E_n = \hbar \omega_c (n + 1/2) \propto (n + 1/2)B\), which depend linearly on the magnetic field (See Fig. 2.11 for comparison). Actually this expression for the Landau levels (LL) coincides with the previous one Eq. (2.74), except for the lowest level which now is

\[
E_0 = 0. \tag{2.77}
\]

It corresponds to the known fact that the lowest Landau for Dirac electron has twice smaller degeneracy as compared with the other Landau levels. These relativistic LLs in graphene have been observed experimentally using scanning tunnelling spectroscopy (STS), which is used to provide information about the density of electrons in a sample as a function of their energy. In this method one shines monochromatic light on the sample and measures the intensity of the transmitted light \([46, 48, 49]\).

2.2.2 Landau levels in bilayer graphene

In this section we present the energy levels and corresponding wavefunctions of an electron in the presence of a homogenous magnetic field in bilayer graphene. Consider a homogeneous magnetic field \(B_0\) normal to the two-dimensional (2D)
Figure 2.11: (a) Landau level as a function of magnetic field. (a) Non-relativistic case with \( E_n \propto (n + 1/2)B \). (b) Dirac electron case with \( E_n \propto \sqrt{nB} \).

plane \((x,y)\) of bilayer graphene. Let us use the Landau gauge for the vector potential \( \mathbf{A}(x) = (0, B_0 x, 0) \) and make the change \( \Pi \to \mathbf{p} + e\mathbf{A} \). The one-electron Hamiltonian for bilayer graphene is

\[
H = \begin{pmatrix}
V_1 & \Pi & t & 0 \\
\Pi^\dagger & V_1 & 0 & 0 \\
t & 0 & V_2 & \Pi^\dagger \\
0 & 0 & \Pi & V_2
\end{pmatrix},
\]

(2.78)

where \( \Pi = v_F[p_x + i(p_y + eA)] \), and \( V_1 \) and \( V_2 \) are the potentials at the two layers and \( t \) is the tunnel coupling between the layers, assumed to be constant. This Hamiltonian is valid near the Dirac point \( K \) or \( K' \). Thus scattering between the \( K \) and \( K' \) valleys is neglected. This scattering was shown \([50]\) to be negligible for fields below \( 10^4 \) T in single-layer graphene; we expect this to be the case in bilayer graphene as well. For more details as well as the motivation why we may neglect trigonal warping, we refer to Ref. \([12]\). To simplify the notation we introduce the length scale \( \ell_B = [\hbar/eB_0]^{1/2} \) and the energy scale \( E_0 = \hbar v_F/\ell_B \). Similar as for the Dirac Hamiltonian, the Hamiltonian in Eq. (2.2.2) commutes with \( p_y \) and therefore is a conserved quantity. This allows us to write \( \Psi(x,y) = \Phi(x) \exp(i k_y y) \) and solve the equation \( H \Psi(x,y) = E \Psi(x,y) \) for the wave function \( \Psi(x,y) = (\phi_a(x), \phi_b(x), \phi_c(x), \phi_d(x))^T \exp(i k_y y) \) with \( T \) denoting the transpose. Then the components of \( \Psi(x,y) \) obey the following set
2.2. IN THE PRESENCE OF MAGNETIC FIELD

Figure 2.12: Observation of Landau levels of massless Dirac fermions. (a) Tunneling spectra plotted against the reduced energy $E/B^{1/2}$. (b) Scaled energy of the aligned peaks plotted against the LL index. (c) Scaled energy levels are linear in $\text{sgn}(n)|n|^{1/2}$. (Figures are from [46])

of coupled differential equations

\[
\begin{align*}
-i(d/dx - (k_y + x))\phi_b + t'\phi_c &= (E - V_1)\phi_a, \\
-i(d/dx + (k_y + x))\phi_a &= (E - V_1)\phi_b, \\
-i(d/dx + (k_y + x))\phi_d + t'\phi_a &= (E - V_2)\phi_c, \\
-i(d/dx - (k_y + x))\phi_c &= (E - V_2)\phi_d.
\end{align*}
\] (2.79)

Setting $V_0 = (V_1 + V_2)/2$, $\Delta V = V_1 - V_2$, $\delta = \Delta V/2$, and $\epsilon = E - V_0$, Eqs. (2.79) can be decoupled. The result for $\phi_a$ is

\[
\left[\frac{d^2}{dz^2} - \frac{z^2}{4} + \frac{\gamma_{\pm}}{2}\right]\phi_a = 0.
\] (2.80)
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Figure 2.13: Quantum Hall effect for massless Dirac fermions. Hall conductivity and longitudinal resistivity of graphene as a function of their concentration at $B = 14T$. (Figures are from [2])

where $\gamma_{\pm} = \epsilon^2 + \delta^2 \pm [(1 - 2\delta\epsilon)^2 + (\epsilon^2 - \delta^2) t'^2]^{1/2}$ and $\sqrt{2}(x + ky) = z$. The solutions of Eq. (2.80) can be written in terms of Weber functions. For an asymptotically vanishing wave function for $z \rightarrow \infty$ we define $\phi_a(z) = e^{-z^2/4}g(z)$ and substitute it in Eq. (2.80). For $\delta = 0$ and using standard power-series procedures we complete the solution and find the energy spectrum

$$\epsilon_{n,\pm} = \pm \left[2n + 1 + \frac{t'^2}{2} \pm \left(\frac{t'^4}{4} + (2n + 1) t'^2 + 1\right)^{1/2}\right]^{1/2}, \quad (2.81)$$

where $n$ is an integer, the Landau-level index. Notice the similarity with the spectrum for single-layer graphene, $E_n = \pm \frac{\hbar v_F}{\ell_B}\sqrt{2(n + 1)}$ or $E_n = \pm \frac{\hbar v_F}{\ell_B}\sqrt{2n}$ and the difference from that for the usual electrons with parabolic energy momentum relation: $E_n = \hbar\omega_c(n + 1/2)$ consisting of equidistant Landau Levels.

For $t \rightarrow 0$, Eq. (2.81) reduces to that of two uncoupled layers with spectrum $E_n = \pm \frac{\hbar v_F}{\ell_B}\sqrt{2n + 1} \pm 1$.

2.2.3 Anomalous quantum Hall effect

In 1981 Klaus von Klitzing and co-workers measured the Hall resistance and the magneto resistance of a two dimensional electron gas (2DEG) [51]. They found that the Hall resistance exhibits plateaus that have quantized values $\hbar/2e^2$ where...
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Figure 2.14: QHE in bilayer graphene. $\sigma_{xy}$ and $\rho_{xx}$ are plotted as a function of $n$ at a fixed magnetic field and temperature. (Figures are from [47])

$n$ is an integer. In 1985 Klaus von Klitzing received the Nobel prize for this discovery. Later in 1981 Laughlin showed [52] that edge effects and broadening of the Landau levels due to disorder have no influence on the accuracy of the Hall quantization. The Landau level at zero energy in graphene separates the electron hole character states from each other. In a magnetic field the resistivity $\rho$ is a tensor given by,

$$\mathbf{J} = e \mathbf{E}, \quad \Rightarrow \quad \rho = \sigma^{-1} \quad (2.82)$$

$$\mathbf{E} = \rho \mathbf{J}.$$
and then the resistivity and conductivity components are

\[ \rho_{xx} = \frac{\sigma_{xx}}{\sigma_{xx}^2 + \sigma_{xy}^2}, \quad \sigma_{xx} = \frac{\rho_{xx}}{\rho_{xx}^2 + \rho_{xy}^2}, \]

\[ \rho_{xy} = -\frac{\sigma_{xy}}{\sigma_{xx}^2 + \sigma_{xy}^2}, \quad \sigma_{xy} = -\frac{\rho_{xy}}{\rho_{xx}^2 + \rho_{xy}^2}. \]  

(2.83)

where \(\sigma_{xx}(\rho_{xx})\) is the longitudinal component and \(\sigma_{xy}(\rho_{xy})\) is the Hall component of the conductivity resistivity. Due to the Lorentz force, the magnetic field produces a Hall voltage \(V_H\) perpendicular to the field and current. The circulating current generates a magnetic flux \(\Phi\) that threads the loop. The current is given by

\[ I = e\frac{\delta U}{\delta \Phi} \]  

(2.84)

where \(U\) is the total energy of the system. When the magnetic flux changes by one flux quantum, \(\delta \Phi = \Phi_0 = \frac{hc}{e}\) the change in energy would be \(\delta U = \pm NeV_H\), where \(N\) is the number of occupied states.

Graphene shows interesting behavior just in the presence of a magnetic field and just with respect to the conductivity-quantization: it displays an anomalous quantum Hall effect with the sequence of steps shifted by \(1/2\) with respect to the standard sequence, and with an additional factor of \(4\). The number of occupied states are \(N = 2 \times (2n + 1)\), since for each Landau level index \(n\) there is in total \(2n\) states for \(K\) and \(K'\) valleys and \(+1\) is due to the zero mode that is shared between two dirac points. Thus, in graphene the Hall conductivity is,

\[ \sigma_{xy} = \frac{I}{V_H} = \pm 4 \left( n + \frac{1}{2} \right) \frac{e^2}{h}. \]  

(2.85)

Factor \(4\) is due to two valley states and two spin states. This unconventional quantum hall effect can even be measured at room temperature, i.e. at roughly \(20^\circ C\) [2]. This anomalous behavior is a direct result of the emergent massless Dirac electrons in graphene [11]. In a magnetic field, their spectrum has a Landau level with energy precisely at the Dirac point. This level is a consequence of the Atiyah-Singer index theorem and is half-filled in neutral graphene, [53] leading to the \(+1/2\) in the Hall conductivity. This result has been experimentally observed [11, 12] as shown in Fig. 2.13.

Quantum Hall effect in bilayer graphene shows that the Hall conductivity is given by,

\[ \sigma_{xy} = \pm 4n \frac{e^2}{h}. \]  

(2.86)
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i.e. with only one of the two anomalies. The integer quantum Hall effect has been observed experimentally in bilayer graphene in Ref. [47] (see Fig. 2.14). Interestingly, concerning the second anomaly, the first plateau at $n = 0$ is absent, indicating that bilayer graphene stays metallic at the Dirac point.

![Figure 2.15: Magnetic field and corresponding vector potential at a distance $z_0 = 0.1$ under the stripe on top for four different configurations. The stripe is magnetized perpendicularly to its plane in (a) and parallel to it in (b). The profiles in (c) are for a current carrying metallic stripe and those in (d) for a superconducting film containing a normal stripe.](image)

2.3 Inhomogeneous magnetic field

One of the most challenging tasks is to learn how to control the electron behavior using electric fields in graphene. This task is made complicated precisely by Klein tunneling according to which Dirac electrons in graphene can tunnel through arbitrarily wide and high electric barriers [32]. Alternatively, one can apply a magnetic field to control the electron motion. It was shown in numerous papers that an inhomogeneous magnetic field can confine electrons described by the Schrödinger
equation [54–56]. The question then arises whether it can confine Dirac electrons in graphene. Up to now semi-infinite magnetic structures, that are homogeneous in one direction, were considered and made the task simpler by converting the problem into an one-dimensional (1D) one [50, 57–64]. In particular, a magnetic confinement of Dirac electrons in graphene was reported in structures involving one [57] or several magnetic barriers [58, 59] as well as in superlattices, without magnetic field for some very special values of the parameters involved [65]. In such structures standard electrons can remain close to the interface and move along so-called snake orbits [55] or in pure quantum mechanical unidirectional states [54]. Given the importance of graphene, it would be appropriate to study this magnetic confinement more systematically by considering different inhomogeneous magnetic field structures such as magnetic barriers, magnetic dot and magnetic superlattices.

There are several methods to create an inhomogeneous magnetic field structure such as growth and patterning techniques, lithographic etching, integration of superconducting materials, including current carrying wires, and recently by applying strain and stress. They result in different magnetic field profiles. Following we describe briefly two of these methods:

### 2.3.1 Ferromagnetic strip

One way is to deposit ferromagnetic strips on top of a graphene layer but such that there is no electrical contact between graphene and these strips (i.e. by adding an oxide layer between them). When one magnetizes the strips along the $x$ direction, cf. Fig. 2.15, by, e.g., applying an in-plane magnetic field, the charge carriers in the graphene layer feel an inhomogeneous magnetic field profile. This profile can be well approximated [54] by $2B_0 z_0 h / (x^2 + z_0^2)$ on one edge of the strip and by $-2B_0 z_0 h / (x^2 + z_0^2)$ on the other, where $z_0$ is the distance between the 2DEG and the strip, and $d$ and $h$ the width and height of the strip (see Fig. 2.15). Simplify the problem, the resulting magnetic field profile can be modeled by two magnetic $\delta$ functions of height $2\pi B_0 h$. Such ferromagnetic strips were deposited on top of a two-dimensional electron gas (2DEG) in a semiconductor heterostructure in Ref. [66].

### 2.3.2 Gauge fields induced by lattice deformation

A recent prediction showed that geometrical deformations of the graphene lattice results in local strains which can induce large pseudo-magnetic fields and produce a pseudo-quantum Hall effect [67–69]. Recently it was reported [34] that nanobubbles grown on a Pt(111) surface induce a pseudo-magnetic field of more than 300
T (see Fig. 2.16). It was shown that on the substrate different graphene bubbles can be observed on different substrates [16, 70] and furthermore by applying an external electric field it is possible to control the curvature [70]. With such large strain-induced pseudo-magnetic fields it becomes possible to control the electronic properties of graphene, which is called "strain engineering". Below we briefly describe the gauge field induced by elastic strain and ripples:

Deformation

The tight-binding Hamiltonian for electrons in graphene when considering that electrons can hop to both nearest and next nearest neighbor atoms can be written in the form [35],

\[
H = -t \sum_{\langle i,j \rangle, \sigma} (a_{i,\sigma}^\dagger b_{\sigma,j} + H.c.) - t' \sum_{\langle i,j \rangle, \sigma} (a_{i,\sigma}^\dagger a_{\sigma,j} + b_{\sigma,i}^\dagger b_{\sigma,j} + H.c.), \tag{2.87}
\]

where \(a_{i,\sigma}(a_{i,\sigma}^\dagger)\) annihilates (creates) an electron with spin \(\sigma\) (\(\sigma = \uparrow, \downarrow\)) on site \(\mathbf{R}_i\) on sublattice \(A\) (an equivalent definition is used for sublattice \(B\)). Applying strain we change the distance or angles between the \(p_z\) orbitals between different sites.
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Then the hopping parameters will change between different sites and a new term will appear in the original Hamiltonian, (2.87)

\[ H_{od} = \sum_{i,j} \left\{ \delta t_{i,j}^{(ab)}(a_i^\dagger b_j + h.c.) + \delta t_{i,j}^{(aa)}(a_i^\dagger a_j + b_j^\dagger b_j) \right\}. \] (2.88)

Fourier transforming of this extra term due to deformation leads to,

\[ H_{od} = \sum_{k,k'} a_{k}^\dagger b_{k'} \sum_{i,\delta_{ab}} \delta t_{i}^{(ab)} e^{i(k-k') \cdot R_i - i\delta_{ab} \cdot k'} + H.c. \]

\[ + (a_{k}^\dagger a_{k'} + b_{k}^\dagger b_{k'}) \sum_{i,\delta_{ab}} \delta t_{i}^{(aa)} e^{i(k-k') \cdot R_i - i\delta_{aa} \cdot k'} \] (2.89)

where \( \delta t_{i,j}^{(ab)} (\delta t_{i,j}^{(aa)}) \) is the change of the hopping energy between orbitals on lattice sites \( R_i \) and \( R_j \) on the same (different) sublattices (we have written \( R_j = R_i + \delta \), where \( \delta_{ab} \) is the nearest-neighbor vector and \( \delta_{aa} \) is the next-nearest-neighbor vector). With projection of the operators close to \( K \) and \( K' \) we find

\[ a_n \simeq e^{-iK \cdot R_n} a_{1,n} + e^{-iK' \cdot R_n} a_{2,n}, \]

\[ b_n \simeq e^{-iK \cdot R_n} b_{1,n} + e^{-iK' \cdot R_n} b_{2,n}. \] (2.90)

To prevent valley scattering we assume \( \delta t_{i,j} \) is smooth over the lattice spacing scale, and does not have a Fourier component with momentum \( K - K' \). Then we will rewrite Eq. (2.89) in real space for the \( K \) point as

\[ H_{od} = \int d^2r \{ A(r) a_{1}^\dagger(r) b_{1}(r) + H.c. + \phi(r)[a_{1}^\dagger(r) a_{1}(r) + b_{1}^\dagger(r) b_{1}(r)]\}, \] (2.91)

for the other valley we have a similar expression except we have to replace \( A \) by \( A^* \), where

\[ A(r) = \sum_{\delta_{ab}} \delta t_{i}^{(ab)}(r) e^{-i\delta_{ab} \cdot K}, \]

\[ \phi(r) = \sum_{\delta_{aa}} \delta t_{i}^{(aa)}(r) e^{-i\delta_{aa} \cdot K}. \] (2.92)

\( A \) is complex due to lack of inversion symmetry for nearest-neighbor hopping and we have,

\[ A(r) = A_x(r) + iA_y(r). \] (2.93)

But due to the inversion symmetry of the two triangular sublattices that make up the honeycomb lattice, \( \phi(r) = \phi^*(r) \). Finally, we can rewrite Eq. (2.91) as

\[ H_{od} = \int d^2r \{ \Psi_1^\dagger(r) \sigma \cdot A(r) \Psi_1(r) + \phi(r) \Psi_1^\dagger(r) \Psi_1(r)\}, \] (2.94)
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The effective magnetic field in the presence of the vector potential is given by 
\[ B = \left( \frac{c}{e v_F} \right) \nabla \times A \]. Due to the existence of the magnetic field we have a broken time-reversal symmetry, although the original problem was time-reversal invariant. This broken time-reversal symmetry is not real since we limited our discussion to one of the Dirac cones. The sign of the strain-induced magnetic field in the two cones is opposite and the two cones are related to each other by time-reversal symmetry and therefore time reversal symmetry will survive in this case.

Elastic strain

The elastic free energy for graphene can be written in terms of the in-plane displacement \( \mathbf{u}(\mathbf{r}) = (u_x, u_y) \) as

\[
F[\mathbf{u}] = \frac{1}{2} \int d^2r \left[ (B - G) \left( \sum_{i=1,2} u_{ii} \right)^2 + 2G \sum_{i,j=1,2} u_{ij}^2 \right], \tag{2.95}
\]

where \( B \) is the bulk modulus, \( G \) is the shear modulus, and

\[
u_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \tag{2.96}
\]
is the strain tensor (\( x_1 = x \) and \( x_2 = y \)).

There are many types of static deformations of the honeycomb lattice that can affect the propagation of Dirac fermions. The simplest one is due to changes in the area of the unit cell due to either dilation or contraction. Changes in the unit-cell area leads to local changes in the density of electrons and, therefore, local changes in the chemical potential in the system. In this case the effective potential given by,

\[
\phi_{dp} = g(u_{xx} + u_{yy}), \tag{2.97}
\]

and their effect is diagonal in the sublattice index.

The nearest-neighbor hopping depends on the length of the carbon bond. Hence, elastic strains that modify the relative orientation of atoms also lead to an effective gauge field, which acts on each \( K \) point separately, as first discussed in relation to carbon nanotubes. Consider two carbon atoms located in two different sublattices in the same unit cell at \( \mathbf{R}_i \). The change in the local bond length can be written as

\[
\delta u_i = \frac{\delta_{ab}}{a} \cdot [\mathbf{u}_A(\mathbf{R}_i) - \mathbf{u}_B(\mathbf{R}_i + \delta_{ab})], \tag{2.98}
\]
The local displacements of the atoms in the unit cell can be related to \( \mathbf{u}(\mathbf{r}) \) by

\[
(\delta_{ab} \cdot \nabla)\mathbf{u} = \kappa^{-1}(\mathbf{u}_A - \mathbf{u}_B), \tag{2.99}
\]
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where $\kappa$ is a dimensionless quantity that depends on microscopic details. Changes in the bond length lead to changes in the hopping amplitude,

$$t_{ij} \approx t_{ij}^0 + \frac{\partial t_{ij}}{\partial a} \delta u_i,$$

and we can

$$\delta t^{ab}(r) \approx \delta u^{(ab)} = \beta \delta u^{(ab)}_a,$$

where

$$\beta = \frac{\partial t^{(ab)}}{\partial \ln(a)}.$$

Substituting Eq. (2.98) into Eq. (2.101) and the final result into Eq. (2.93), we find

$$A^{(s)}_x = \frac{3}{4} \beta \kappa (u_{xx} - u_{yy}),$$

$$A^{(s)}_y = \frac{3}{2} \beta \kappa u_{xy},$$

where $\beta/v_F \approx a^{-1} \sim 1 \text{ Å}^{-1}$. In conclusion, changes in the hopping amplitude induce a vector $A$ and scalar $\phi$ potential in the Dirac Hamiltonian.

Ripples

The graphene membrane $s(r)$ placed on a substrate will follow the geometry of the substrate $h(r)$. With bending graphene the inter atomic distance in graphene decrease and the $p_z$ orbitals rotate with respect to each other and a rehybridization between $\pi$ and $\sigma$ orbitals will occur. Bending the graphene sheet leads to a modified hopping between different sites of the form, $\delta t_{ij} \approx -t_{ij}^0 \frac{\nabla h(r_i)}{2}$, where $u_{ij}$ is the strain tensor and $t_{ij}^0$ is the hopping parameter for flat graphene. It was shown that such deformation can induce an effective vector potential as,

$$A^h_x = -\frac{3E_{ab}a^2}{8} [(\partial_x^2)^2 - (\partial_y^2)^2] h$$

$$A^h_y = \frac{3E_{ab}a^2}{4} (\partial_x^2 + \partial_y^2) \partial_x \partial_y h,$$

(2.104)
Abstract. In this chapter the technique of beam optics is applied to the description of the wave function of Dirac electrons. This approach is illustrated by considering electron transmission through simple non-homogeneous structures, such as flat and bent p-n junctions and superlattices. We found that a convex p-n junction compresses the beam waist, while a concave interface widens it without losing its focusing properties. At a flat p-n junction the waist of the transmitted Gaussian beam can be narrowed or widen depending on the angle of incidence. A general condition is derived for the occurrence of beam collimation in a superlattice.

3.1 Introduction

The possibility to perform experiments at very low temperatures with pure materials stimulated investigations of sophisticated quantum properties of electron systems, especially the peculiarities of the electron wave functions, their control and search of analogies with electromagnetic waves. For instance, the meta-material character of p-n-structures in graphene [36] was pointed out, and focusing of electronic waves was proposed [71]. The meta-material properties of the above mentioned p-n-structures resulted in the expectancy of controlling the electron wave function, in particular, the width of electron beams by means of a superlattice. This behavior is known as collimation. Recently it was shown that superlattices on graphene can be fabricated in various ways [72–75] what induced a large theoretical activity in this field, such as the investigation of electron focusing [76–78], collimation of electrons and photons [79–83], and interference [84] in a two-dimensional electron gas.

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CHAPTER 3. APPLICATION OF OPTICAL BEAMS TO ELECTRONS IN GRAPHENE

Qualitatively, the meta-material properties of p-n-junctions in graphene can be understood by inspecting classical trajectories, or using ray optics as it is called for the case of electromagnetic phenomena. Meanwhile the quantitative description of these properties can be achieved by laborious numerical simulation of the Schrödinger and Dirac equations (similar to the Maxwell equations for describing electromagnetic phenomena).

In photonics an intermediate approach based on beam optics \[85\] has been widely used, in particular in laser physics. Beam optics is based on the simplicity of ray optics but with the inclusion of essential phenomena such as diffraction and interference. When compared to mechanics it corresponds to the so called quasi-classical approach.

The aim of this section is to transfer the technique of Gaussian beams developed in optics to the description of Dirac electron wave functions, and to illustrate their application in electron propagation through the most simple non-homogenous structures, such as flat and bent p-n-junctions and superlattices. The main advantage of the present approach as compared with the previous calculations is its simplicity and the fact that most of the results can be obtained analytically.

3.2 Gaussian beams in optics

We first review the basic properties of Gaussian beams in optics that are essential when solving the Dirac equation for the corresponding electron beams in graphene.

Following Saleh’s textbook \[85\], Gaussian beams are known as solutions of the 3D (three dimensional) Helmholtz equation

\[
\left( \nabla^2 + k^2 \right) u(\mathbf{r}) = 0
\]

in the form of paraxial waves

\[
u(\mathbf{r}) = A(\mathbf{r}) e^{ikx}
\]

propagating along the \(x\)-axis. The envelope \(A(\mathbf{r})\) is assumed to be a slowly varying function over distances of the order of the wavelength \(\lambda = 2\pi/k\). This envelope satisfies the paraxial Helmholtz equation

\[
\left( \nabla^2_\perp + 2ik \frac{\partial}{\partial x} \right) A(\mathbf{r}) = 0
\]

where \(\nabla^2_\perp = \partial^2/\partial y^2 + \partial^2/\partial z^2\) stands for the 2D Laplacian in the plane perpendicular to the direction of beam propagation. Inspecting terms in the above equation
and comparing them with the terms in Eq. (3.1) we conclude that the validity of the paraxial approximation can be formally expressed as

\[ k^{-1} \frac{\partial}{\partial x} A = \gamma A \ll A, \quad \partial^2_\perp A \sim k \partial_x A \sim \gamma k^2 A. \]  

(3.4)

So, in the paraxial approximation terms of order \( \gamma \) are taken into account while terms of order \( \gamma^2 \) are omitted, or only the leading terms are taken into account.

Making use of the analogy with the Green’s function of the diffusion equation for imaginary time (e.g. \( t \to ix/2k \)), the solution of Eq. (3.3) can be presented as

\[ A(r) = \frac{A}{x-w} \exp \left\{ \frac{ik\rho^2}{2(x-w)} \right\} \]  

(3.5)

where \( \rho = \sqrt{y^2 + z^2} \) is the radial coordinate in the \( yz \)-plane, and

\[ w = u + iv, \]  

(3.6)

is some complex shift of the argument which can be included due to the translational symmetry of Eq. (3.3). The above complex constant allows us to obtain a finite beam solution in the \( yz \)-plane.

Usually the denominator in the argument of the exponent is decomposed as follows:

\[ \frac{1}{x-w} = \frac{1}{x-u-iv} = \frac{x-u}{(x-u)^2 + v^2} + \frac{iv}{(x-u)^2 + v^2} = \frac{1}{R(x-u)} + \frac{2i}{kW^2(x-u)}, \]  

(3.7)

where the symbol \( W(x) \) stands for the beam radius and \( R(x) \) — for the wavefront radius of curvature. The smallest beam radius

\[ W_0 = W(0) = \sqrt{\frac{2v}{k}} \]  

(3.8)

is called the beam waist, while the parameter \( 2v \) characterizes the depth of focus and is called the confocal parameter. The parameter \( u \) is just the position of the waist on the \( x \)-axis. All these quantities are shown in Fig. 3.1. The beam radius \( W(x) \) is shown by the red curve. In the limiting case of \( x \to \pm \infty \) it approaches the two blue lines indicating the angular divergence of the beam

\[ \theta_0 = \frac{2}{kW_0}. \]  

(3.9)
Taking into account the condition (3.4) it is easy to conclude that the paraxial approximation is valid when

$$\frac{\partial A}{\partial x} \ll kA, \quad \text{or} \quad \theta_0 \ll 1,$$

namely, in the case of weakly diverging beams.

The intensity of the beam can be calculated in a standard way as

$$I(\rho, x) = |u(r)|^2 = \frac{I_0}{(x-u)^2 + v^2} \exp \left[ -\frac{k \rho^2 v}{(x-u)^2 + v^2} \right]$$

$$= I_0 \left[ \frac{W_0}{W^2(x-u)} \right]^2 \exp \left[ -\frac{2\rho^2}{W^2(x-u)} \right],$$

(3.11)

where $I_0 = |A|^2/v^2$ characterizes the total optical power $(\pi W_0^2 I_0/2)$ of the beam. The above equation actually justifies the name of the beam’s radius $W(x)$.

All these expressions can be straightforwardly applied to 3D electron beams that are described by the Schrödinger equation. For free electrons this equation coincides with the Helmholtz equation (3.1) if one takes into account the definition of the electron energy, namely, $E = \hbar^2 k^2 / 2$.

### 3.3 Gaussian beams applied to the Dirac equation

Now we turn to the Dirac-Weyl equation that is used in a continuum description of electrons and holes in graphene or for electrons in topological insulators. In the stationary case this equation can be presented in the form of a Schrödinger equation

$$(H - E) \Psi(r) = 0,$$

(3.12)

with the following dimensionless 2D Hamiltonian

$$H = -i \begin{pmatrix} 0 & \partial/\partial x - i \partial/\partial y \\ \partial/\partial x + i \partial/\partial y & 0 \end{pmatrix}.$$

(3.13)
3.3. GAUSSIAN BEAMS APPLIED TO THE DIRAC EQUATION

All dimensions can be excluded, say, measuring distances in lattice constant $a_0$ units, time — in $a_0/v_F$ units, and energy — in $\hbar v_F/a_0$ units (here $v_F$ is the Fermi velocity — the single parameter characterizing the Dirac Hamiltonian for particles with zero rest mass).

Eq. (3.12) has to be satisfied by the two component eigenfunction

$$\Psi(r) = \Psi(x, y) = \begin{pmatrix} F(r) \\ G(r) \end{pmatrix},$$

where the components obey the following set of equations:

$$\left( \frac{\partial}{\partial x} - i \frac{\partial}{\partial y} \right) G(r) = iEF(r), \quad (3.15a)$$

$$\left( \frac{\partial}{\partial x} + i \frac{\partial}{\partial y} \right) F(r) = iEG(r). \quad (3.15b)$$

Substituting the component $G(r)$ (expressed from the second equation) into the first one we arrive at the equation for the single $F(r)$ component

$$\left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + E^2 \right) F(r) = 0. \quad (3.16)$$

which coincides with the 2D Helmholtz equation (3.1) or the Schrödinger equation for standard electrons if we take into account the electron and hole energy dependence

$$E = \pm k \quad (3.17)$$

in graphene.

The different dimensionality of the problem slightly changes the paraxial equation for the envelope functions introduced as

$$F(r) = e^{ikx} f(r), \quad G(r) = e^{ikx} g(r) \quad (3.18)$$

for the beam propagating along the $x$ axis. Now instead of Eq. (3.3) we have to write down the following equation for the first envelope function component:

$$\left( \frac{\partial^2}{\partial y^2} + 2ik \frac{\partial}{\partial x} \right) f(r) = 0. \quad (3.19)$$

The solution of the above equation, in analogy with the Gaussian beam in optics (3.5), can be presented as

$$f(r) = \frac{A}{\sqrt{x-w}} \exp \left\{ -\frac{iky^2}{2(x-w)} \right\}. \quad (3.20)$$
We see that the exponents that define the main properties of the Gaussian beam are the same in both Eqs. (3.20) and (3.5). Only the prefactors are different that is caused by the peculiarities of the Green’s function of the 1D diffusion equation.

The second envelope function component can be obtained using Eqs. (3.15b) and (3.18). It reads

\[ g = -\frac{i}{E} e^{-ikx} \left( \frac{\partial}{\partial x} + i \frac{\partial}{\partial y} \right) e^{ikx} f \]

\[ = -\frac{i}{E} (ik + \partial_x + i \partial_y) f \approx k \frac{E}{f}. \] (3.21)

We shall restrict our consideration by taking into account only the last approximate expression, or including just the leading term, what according to Eq. (3.4), is the essence of the paraxial approximation. Thus, the Gaussian beam propagating along the \( x \)-axis, being the approximate solution of the Dirac equation, can be presented as

\[ \Psi(r) = A e^{ikx} \sqrt{x-w} \left( \frac{k}{E} \right) \exp \left\{ \frac{iky^2}{2(x-w)} \right\}. \] (3.22)

If the beam propagates in some other direction its wave function can be obtained from Eq. (3.22) by properly rotating the \((x, y)\) coordinates and the spinor part of the wave function as well.

### 3.3.1 Transmission of electron beam through a bent potential step

For illustrative purposes we will use the expressions obtained in the previous section for Dirac electron Gaussian beams and apply them to the penetration of these electrons into a bent electric potential step in graphene. We assume that the \( xy \)-plane is divided into two parts by the circular interface

\[ (x-R_0)^2 + y^2 = R_0^2. \] (3.23)

In the vicinity of a narrow Gaussian beam propagating along the \( x \)-axis it can be replaced by the following parabolic curve:

\[ x = \frac{y^2}{2R_0}. \] (3.24)

where the symbol \( R_0 \) stands for the radius of the bent potential interface. We assume that the homogeneous electric potential of strength \( V \) is applied on the right side of this interface while it is zero on the left hand side. This barrier is shown schematically in Fig. 3.2 together with the band structure of graphene.
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Figure 3.2: Potential barrier and the band structure of graphene.

We assume that the incident electron beam with energy \(E = k_i > 0\)

\[
\Psi_i(r) = \frac{A_i e^{i k_i x}}{\sqrt{x-w_i}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \exp \left\{ \frac{i k_i y^2}{2(x-w_i)} \right\}
\]

(3.25)
is coming from the left side in region I. It corresponds to the point 1 indicated by the red full circle in Fig. 3.2. So, in the case of positive \(R_0\) the interface (3.24) corresponds to a convex lens.

We assume that the energy of the incident electron is smaller than the potential height \((E < V)\). Due to conservation of energy and chirality the electron in the barrier corresponds to point 2 (full violet circle) in the energy spectrum shown in Fig. 3.2. Points 3 and 4 shown by hollow circles do not contribute in the paraxial approximation due to the above mentioned conservation of chirality.

So, the wave function on the right side of the barrier II reads

\[
\Psi_t(r) = \frac{A_t e^{i k_t x}}{\sqrt{x-w_t}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \exp \left\{ \frac{i k_t y^2}{2(x-w_t)} \right\},
\]

(3.26)
where

\[ k_t = E - V < 0. \]

(3.27)
The incident (3.25) and transmitted (3.26) beams have to satisfy the boundary condition at the interface (3.24) that reads

\[
\frac{A_i e^{i k_i y^2/2R_0}}{\sqrt{y^2/2R_0 - w_i}} \exp \left\{ \frac{i k_i y^2}{2(y^2/2R_0 - w_i)} \right\} = \frac{A_t e^{i k_t y^2/2R_0}}{\sqrt{y^2/2R_0 - w_t}} \exp \left\{ \frac{i k_t y^2}{2(y^2/2R_0 - w_t)} \right\}.
\]

(3.28)

Taking into account the weak divergence of the Gaussian beam and assuming a large radius for the bent interface \((R_0 \gg \lambda)\) the above expression can be simplified.
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by neglecting \( y^2/2R_0 \) terms in comparison with the \( w_{i,t} \) terms in the denominators. This replaced Eq. (3.28) by the following equation:

\[
\frac{A_i}{\sqrt{-w_{i}}} \exp \left\{ ik_i y^2 \left[ 1/2R_0 - 1/2w_{i} \right] \right\} = \frac{A_t}{\sqrt{-w_{t}}} \exp \left\{ ik_t y^2 \left[ 1/2R_0 - 1/2w_{t} \right] \right\} .
\]

(3.29)

As this equation has to hold for any \( y \) value at the interface, the following condition should be satisfied:

\[
k_i \left( \frac{1}{R_0} - \frac{1}{w_{i}} \right) = k_t \left( \frac{1}{R_0} - \frac{1}{w_{t}} \right).
\]

(3.30)

Note that this is the main equation for lenses and mirrors in optics.

In the case of a flat interface (i.e. \( R_0 = \infty \)) the above equation reduces to the more simple one

\[
k_i/w_i = k_t/w_t,
\]

(3.31)

or

\[
w_t = -\kappa w_i, \quad \kappa = \frac{V - E}{E} > 0.
\]

(3.32)

Consequently, the position of the waist of the incident and transmitted beams (\( u_i \) and \( u_t \) respectively) have different signs as illustrated in Fig. 3.3 where the radii of corresponding beams are shown by red and blue solid curves.

Figure 3.3: Beam penetration into the flat potential step at \( x = 0 \) for \( E < V \).

It is remarkable that the flat interface doesn’t influence the radius of waist. Indeed, according to Eqs. (3.8) and (3.31) we have

\[
W_{0t} = \sqrt{\frac{2v_{t}}{k_t}} = \sqrt{\frac{2v_i}{k_i}} = W_{0i},
\]

(3.33)
while the focusing properties of this interface, namely, the divergence of the beam according to Eq. (3.9) can be enlarged as seen by

$$\theta_{0t} = \frac{2}{k_t W_{0t}} = \frac{k_i}{k_t} \theta_{0i} = \frac{1}{\kappa} \theta_{0i}$$  \hspace{1cm} (3.34)

when the energy of the incident electron approaches the top of the barrier. Notice that when the electron energy becomes larger than the potential height, the interface looses its focusing possibility because in this case \( \kappa < 0 \), and both beam waists are at the same side of the interface. Now the beam diverges after the penetration into the barrier as illustrated in Fig. 3.4.

![Figure 3.4: Diverging beam when penetrating the flat potential step at \( x = 0 \) when \( E > V \).](image)

One can change the waist of the beam in the barrier by using a bent interface. In this case assuming that the waists of both beams are not close to the interface (i.e. \( |u_i| \gg v_i \) and \( |u_t| \gg v_t \)), we can rewrite Eq. (3.7) as

$$\frac{1}{w_{i,t}} \approx \frac{1}{u_{i,t}} - \frac{iv_{i,t}}{u_{i,t}^2},$$  \hspace{1cm} (3.35)

and inserting it into Eq. (3.30), and separating its real and imaginary parts we obtain two equations

$$k_i \left( \frac{1}{R_0} - \frac{1}{u_i} \right) = k_t \left( \frac{1}{R_0} - \frac{1}{u_t} \right),$$  \hspace{1cm} (3.36a)

$$\frac{k_i v_i}{u_i^2} = \frac{k_t v_t}{u_t^2},$$  \hspace{1cm} (3.36b)

which characterize the transition of the Gaussian beam through the bent interface. Now using Eqs. (3.8) and (3.36b) the waist ratio becomes

$$\frac{W_{0t}}{W_{0i}} = \sqrt{\frac{k_i v_i}{k_t v_t}} = \frac{k_i u_t}{k_t u_i}.$$  \hspace{1cm} (3.37)
Using Eq. (3.36a) we can express the ratio $u_i/u_t$ as

$$\frac{u_i}{u_t} = \frac{k_i}{k_t} \left[ 1 - \left( 1 - \frac{k_i}{k_t} \right) \frac{u_i}{R_0} \right],$$  \hspace{1cm} (3.38)

and we obtain the following equation for the ratio of the beam waists:

$$\frac{W_{0t}}{W_{0i}} = \left(1 - \frac{Vu_i}{ER_0}\right)^{-1}. \hspace{1cm} (3.39)$$

We see that in the case of a diverging beam coming from the left side ($u_i < 0$) the convex ($R_0 > 0$) interface compress the beam waist similar as the action of a convex lens in optics, while a concave interface ($R_0 < 0$) in contrast widens it without losing its focusing ability.

### 3.3.2 Reflection of the oblique beam

Now we consider a standard optics problem — reflection and transmission through the interface of two different media. The layout for the case of graphene is shown in Fig. 3.5. On the right half-plane (shown in yellow) there is a barrier — the homogeneous electric potential of strength $V$, while on the left half-plane the potential is taken zero. The vector $k_i$ indicates the direction of the incident beam characterized by the incident angle $\theta_i$. The most simple way to construct the wave function that corresponds to that incident beam is to use the coordinate system $(x_i, y_i)$ rotated by the angle $\theta_i$, namely,

$$x_i = x \cos \theta_i + y \sin \theta_i, \hspace{1cm} (3.40a)$$

$$y_i = -x \sin \theta_i + y \cos \theta_i, \hspace{1cm} (3.40b)$$

Figure 3.5: Reflection and transmission at an interface.
in which the vector $k_i$ is located along the $x_i$-axis. Thus, taking into account that the spinor has to be rotated as well and denoting $E = |k_i|$ we rewrite Eq. (3.25) as follows:

$$\Psi_i(r) = A_i e^{iE x_i} \frac{1}{\sqrt{x_i - w_i}} \exp \left\{ \frac{iE y_i^2}{2(x_i - w_i)} \right\}. \quad (3.41)$$

In an analogous way denoting the reflection angle by the symbol $\theta_r$ and rotating coordinates by the angle $\pi - \theta_r$ in Eq. (3.25), we obtain the wave function of the reflected beam

$$\Psi_r(r) = A_r e^{iE x_r} \frac{1}{\sqrt{x_r - w_r}} \exp \left\{ \frac{iE y_r^2}{2(x_r - w_r)} \right\}. \quad (3.42)$$

The wave function of the transmitted beam is similar to Eq. (3.41) where the index $i$ has to be replaced by $t$, and the energy $E$ by the electron energy in the barrier $E - V$.

Now satisfying the boundary condition at the interface ($x = 0$) we obtain the equation:

$$e^{iE y \sin \theta_i} \frac{1}{e^{i\theta_i}} \frac{A_i \Phi_i(E)}{\sqrt{y \sin \theta_i - w_i}} + e^{iE y \sin \theta_r} \frac{1}{-e^{-i\theta_r}} \frac{A_r \Phi_r(E)}{\sqrt{y \sin \theta_r - w_r}} = e^{i(E - V) y \sin \theta_t} \frac{1}{e^{i\theta_t}} \frac{A_t \Phi_t(E - V)}{\sqrt{y \sin \theta_t - w_t}}, \quad (3.43)$$

where the following short notation is used:

$$\Phi_{\alpha}(E) = \exp \left\{ \frac{iE y^2 \cos^2 \theta_\alpha}{2(y \sin \theta_\alpha - w_\alpha)} \right\}. \quad (3.44)$$

The above equation has to be satisfied for any $y$ value at the interface. This implies that the arguments of the exponents that include the coordinate $y$ have to be equal. So, applying this procedure to the first exponent in all three terms of Eq. (3.43) we obtain the following equations:

$$E \sin \theta_i = E \sin \theta_r = (E - V) \sin \theta_t. \quad (3.45)$$

This is nothing else then Snell’s law:

$$\theta_r = \theta_i, \quad \sin \theta_t = -\frac{1}{\kappa} \sin \theta_i. \quad (3.46)$$
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If \( E < V (\kappa > 0) \) we have a negative angle of refraction \( (\theta_t < 0) \) as in the case of a metamaterial.

To equate the arguments of the second exponent in each of the three terms of Eq. (3.43) as given by Eq. (3.44) is hardly possible due to the non-trivial \( y \)-dependence of the nominator of this expression and of the denominator as well. Therefore, we have to invoke some approximations. For this purpose we draw our attention to definition (3.6) and Eq. (3.7) from which it follows that the term \( y \sin \theta_\alpha \) that actually doesn’t exceeds the beam radius competes with the term \( u_\alpha \) that indicates the distance from the interface to the beam’s waist. Consequently, if the waist isn’t close to the interface, namely, if the above distance \( u_\alpha \) is larger than the radius of the beam characterized by the value \( v_\alpha \) the term \( y \sin \theta_\alpha \) can be neglected as compared with the shift \( w_\alpha \). Making use of this approximation and equating the arguments of the \( \Phi_\alpha(E) \) type exponents in all three terms of Eq. (3.43) we obtain the following equations:

\[
\frac{E \cos^2 \theta_i}{w_i} = \frac{E \cos^2 \theta_r}{w_r} = \frac{(E - V) \cos^2 \theta_t}{w_t}, \tag{3.47a}
\]

\[
\left(1 - e^{i \theta_t}ight) \frac{A_t}{\sqrt{-w_i}} + \left(1 - e^{-i \theta_r}\right) \frac{A_r}{\sqrt{-w_r}} = \left(1 - e^{i \theta_t}\right) \frac{A_t}{\sqrt{-w_t}}. \tag{3.47b}
\]

These equations completely solve the beam reflection problem. Eq. (3.47a) enables to define \( w_r \) and \( w_t \), namely, the basic characteristics of reflected and transmitted beams:

\[
w_r = w_t = -\frac{w_i \cos^2 \theta_i}{\kappa \cos^2 \theta_t}. \tag{3.48}
\]

The first equality indicates that the reflected beam has the same characteristics as the incident one, actually its a continuation with the same divergence rate. The second equality enables to estimate the waist of the transmitted beam. It reads

\[
\frac{W_{0t}^2}{W_{0i}^2} = -\frac{1}{\kappa} \frac{v_t}{v_i} = \frac{\cos^2 \theta_t}{\cos^2 \theta_i}, \tag{3.49}
\]

and consequently

\[
\frac{W_{0t}}{W_{0i}} = \frac{\cos \theta_t}{\cos \theta_i}. \tag{3.50}
\]

Thus the waist of the transmitted beam can be increased (or decreased) as compared with the incident beam depending on the angle of incidence.

And at last Eq. (3.47b) enables to evaluate the intensities of the transmitted and reflected beams. This equation is actually the same equation for homogeneous
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beams described by the corresponding exponents (see, for instance, a similar calculations in Ref. [32]) with a single exception, namely, the additional factors $w_α$ that actually takes into account the change of the beam waist during the reflection or transmission.

3.3.3 Beam collimation in superlattice

Using Eq. (3.31) that describes the transformation of the main beam parameters when passing through the flat p-n-interface it becomes now easy to trace the transmission of the electron beam through the superlattice that is composed as a periodic structure of the above interfaces. Such a superlattice is schematically shown in Fig. 3.6. We assume that this superlattice consists of alternating n-regions of length $s$ (shown in white) with zero potential and p-regions (or barriers) of length $d$ (shown in yellow) with electric potential $V$. The radius of the electron beam propagating perpendicular to these superlattice layers is shown by solid red and blue curves in Fig. 3.6. The corresponding dashed lines indicate the divergences of various beam parts. The horizontal dashed green line shows the position of the beam waist that according to Eq. (3.33) conserves its value in the case of the considered flat interfaces.

As the waist value is conserved during electron transmission through the interface indicated by the number $n$, the main variables that characterizes this transmission are $a_n$ and $b_n$ which are the distances of incoming and outgoing beam waists from that interface (see Fig. 3.6). According to Eq. (3.32) they are related by

$$b_n = -a_n\kappa, \quad \text{and} \quad a_n = -b_n/\kappa.$$  \hspace{1cm} (3.51)

The single important thing that has to be taken into account is that these relations have to be used in the coordinate system attached to the considered interface. Thus, we can write down the following set of equations connecting the waist positions in
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Various superlattice layers:

\[ b_n = -\kappa a_n, \]  

\[ a_{n+1} - s = -\frac{1}{\kappa}(b_n - d), \]  

or

\[ a_{n+1} = a_n + \left(\frac{d}{\kappa} - s\right). \]  

The solution of this simple equation reads

\[ a_n = a_1 + \left(\frac{d}{\kappa} - s\right)(n - 1). \]  

It is remarkable that Eq. (3.53) and its solution (3.54) hold even in the case when the waist positions are outside the layers that contact the interface under consideration. Thus, it follows from Eq. (3.54) that in general the distance of the beam waist from the interface increases when \( n \to \infty \), and consequently, the electron beam diverges. The single exception is the case when the electron energy satisfies the following condition:

\[ d = \kappa s, \quad \text{or} \quad E = \frac{s}{s + d}V. \]  

This is actually the condition of electron beam collimation by means of a superlattice composed of alternating p-n- and n-p-interfaces.

It is remarkable that the above condition could be formulated within the framework of a quasi-classical approach and actually isn’t related to band parameters. Previously the collimation of electrons was related to their spectrum. It was argued that the presence of flat regions in the electron energy-momentum spectrum favors collimation [81, 86] of beams propagating in the direction perpendicular to those flat regions. The disadvantage of the latter technique was the very small superlattice period (of order nanometers) and rather large barrier heights (of order tenth’s of eV) that was required in order to observe collimation (see for instance Ref. [80]). Note that the presented quasi-classical Gaussian beams are free of this disadvantage.

3.3.4 Conclusions

We rewrote the Gaussian beam expressions used in optics and adjusted them for the description of Dirac electrons. The application of Gaussian beams was illustrated by considering electron beam transmission through simple nonhomogeneous structures.
3.3. GAUSSIAN BEAMS APPLIED TO THE DIRAC EQUATION

It was shown that although a p-n-interface in graphene exhibits a negative refraction for an electron beam, like in an optical metamaterial, it doesn’t influence the electron beam waist which is the essential feature of any lens focusing of optical rays. A contraction of the beam waist, however, is possible if one uses a bent p-n-interface which actually resembles a real lens.

Looking for possible electron beam collimation we applied our results to electron propagation in a superlattice, and obtained a general condition under which such a collimation can be realized. We showed that collimation is possible in the case of larger lattice constants and smaller barrier heights than previously predicted.
Fabry-Pérot resonances in graphene microstructures: influence of a magnetic field

Abstract. Fabry-Pérot resonances in the transmission through single and double, graphene-based barriers (of height $V$) and wells are investigated and their dependence on an applied perpendicular magnetic field. For rectangular barriers the conductance decreases with increasing magnetic field while the resonances weaken (become more pronounced) with increasing magnetic field for $E_F < V$ ($E_F > V$). The position of the resonances exhibit a linear shift with magnetic field which move to lower (higher) energy for $E_F < V$ ($E_F > V$). Compared to semielliptic- or gaussian-shaped barriers they show a smaller number of resonances in the absence of a magnetic field and an overall lower conductance but the resonant structure is more pronounced. The conductance of asymmetric double barriers show two major regions of resonances while the symmetric ones show one, that of three asymmetric barriers three, and so on.

4.1 Introduction

One important aspect of the electronic transmission through quantum structures is the Fabry-Pérot resonances which are a consequence of the wave nature of the electron. Recently it was shown that such resonances exist for different semi-infinite structures such as barriers or double barriers (wells) [87–90]. In addition, n-p, n-p-n, and p-n-p junctions have been fabricated [90–99] in which Klein tunneling and Fabry-Perot resonances were observed [91, 92]. In such devices the height of the potential barriers and the position of the Fermi level could be tuned by gate potentials. In Ref. [92] the metallic gates that induced the potential barriers were about
50 − 100 nm separated from the graphene layer and the length of the Fabry-Perot cavity was about 740 nm. With such devices FP resonances were observed in the resistance oscillations. In such p-n junctions the top gate lays on an insulating layer that can decrease the mobility of graphene. In order to avoid this problem one can fabricate p-n-p graphene structures using suspended air-bridge top gates [93].

The recent theoretical work of Ref. [90] studied the dependence of Fabry-Pérot resonances on magnetic field in the presence of a parabolic gate potential [93]. In such a system (for \( E > 0 \)) the electron-like states inside the potential region give rise to the FP resonances. Here we consider a potential barrier which has both electron-like \( (E > V) \) and hole-like \( (E < V) \) states for \( E > 0 \), and compare the effect of a magnetic field on the FP resonances of these two different states.

We consider single and multiple rectangular barrier structures and concentrate on resonances in the transmission and conductance and their dependence on magnetic field.

### 4.2 Potential barrier as a Fabry-Perot interferometer

The low-energy quasi-particles (electrons and holes) in graphene are described by the following Dirac type Hamiltonian

\[
H = v_F \sigma \cdot \mathbf{p} + V, \tag{4.1}
\]

where \( p_\nu = -i\hbar (\partial / \partial x_\nu) \) is the momentum operator, \( v_F \) the Fermi velocity, and \( \sigma \) the Pauli matrices. We assume \( V = V(x) \) to be one-dimensional potential. Then the equation \( H \Psi(x, y) = E \Psi(x, y) \) admits spinor solutions of the form

\[
\Psi(x, y) = \left( \begin{array}{c} \psi_I(x, y) \\ \psi_{II}(x, y) \end{array} \right). \tag{4.2}
\]

Following our calculations in Sec. 2.1.4 we find the transmission probability for a single barrier [32],

\[
T = \frac{\cos^2 \theta \cos^2 \varphi}{\cos \mu \cos \theta \cos \varphi + \sin^2 \mu (1 - s s_0 \sin \theta \sin \varphi)^2}, \tag{4.3}
\]

where \( \mu = k_2 W \). Substituting \( \mu = n\pi \) in Eq. (4.3) we obtain the energies \( E \) at which the resonances occur (i.e., \( T = 1 \))

\[
E = V \pm [k_y^2 + n^2 \pi^2 / W^2]^{1/2}. \tag{4.4}
\]

We have at least one resonance if

\[
W > \pi / V. \tag{4.5}
\]
4.2. POTENTIAL BARRIER AS A FABRY-PEROT INTERFEROMETER

![Figure 4.1](image)

Figure 4.1: (a) Schematics of the transmission through a barrier of width $W$. (b) The wave function of a localized state in the yellow region of (c). Dispersion relation $E(k_y)$ in the presence of a potential barrier. The dotted curves show the analytical dispersion relation (4.4) for $W = 100$ nm and $V = 100$ meV. The four qualitatively different transmission regions are explained in the text.

As shown in Fig. 4.1(c) there are four different regions. In the green region $k_1$ and $\kappa$ are real and the solutions inside and outside the barrier are traveling waves and due to Klein tunnelling we have a high transmission probability where the transmission maxima given by Eq. (4.4) and shown in Fig. 4.2(a) by the dashed curves. We can divide this region in two parts: $E > V/2$ and $E < V/2$. For $E > V/2$ all maxima terminate in the free-electron spectrum $E = V \pm k_y$ that is shifted by the barrier potential. For $E < V/2$ though all maxima (dashed curves) cut the free-electron spectrum $E = \pm k_y$. The corresponding crossing points can be found by substituting $k_y^2 = E^2$ in Eq. (4.4). We can also obtain the confinement state by using the localized solutions for the electron outside the barrier. The spectrum of the bound states are obtained from the solution of the transcendental equation [99]
Figure 4.2: (a) Contour plot of the transmission vs energy $E$ and wave vector $k_y$. The dotted curves show the analytical dispersion relation (4.4) for $W = 100$ nm and $V = 100$ meV. (b) Transmission vs $k_x$ and $k_y$ for $W = 100$ nm and $V = 100$ meV. The dashed curve shows the position of $E = V/2$. (c)-(d) Contour plot of the transmission for constant energies $E = 25$ meV and $E = 50$ meV, respectively as a function of $W$ and $k_y$.

Indeed, for $\kappa W = n\pi$, Eq. (4.6) entails $k_1 \to 0$, $k_2^2 = E^2$ and we can rewrite Eq. (4.4) as

$$E = \frac{V}{2} - \frac{n^2\pi^2}{2W^2V}. \quad (4.7)$$

In the blue region of Fig. 4.1(c) $k_1$ is real but $k_2$ is imaginary. Then we have traveling wave solutions outside the barrier but inside it the solutions are evanescent waves. This is similar to the case of a standard electron with energy $E < V$ passing through a potential barrier with small transmission probability.

In the yellow region of Fig. 4.1(c) $k_2$ is real but $k_1$ is imaginary. This results in traveling wave solutions inside the barrier and evanescent ones outside it, that is, we have states bound to the potential barrier see Fig. 4.1(b). In fact, we have angular confinement of the waves inside the barriers if the following inequalities
4.2. POTENTIAL BARRIER AS A FABRY-PEROT INTERFEROMETER

Figure 4.3: (a) Contour plot of the transmission through a single barrier vs its height $V$ and wave vector $k_y$ for $W = 100$ nm. (b) Same as in (a) but in the presence of a magnetic field $B = 100$ mT.

The energies of the bound states coincide with those at which the transmission maxima occur and are given by Eq. (4.7). Finally, in the white region both $k_1$ and $k_2$ are imaginary. The corresponding solutions are evanescent waves and the electron cannot tunnel through the barrier.

A few contour plots of the transmission are shown in Figs. 4.2 and 4.3, see the caption for details on the parameters. One can clearly see the Fabry-Pérot resonances in all cases. A fundamental difference with the corresponding results for Schrödinger-type electrons is that the Fabry-Pérot resonances now depend on
CHAPTER 4. FABRY-PÉROT RESONANCES IN GRAPHENE MICROSTRUCTURES: INFLUENCE OF A MAGNETIC FIELD

$k_y$ as well instead of only the wave vector $k_x$. In Fig. 4.3 we show a contour plot of transmission as a function of momentum and potential height. The potential height can be controlled by an applied top gate [93].

Next we consider a double barrier and start with a symmetric one, i.e., one in which the barriers have the same height and width and are separated by a distance $W_s$. The wave vector $k_x$ is the same in the regions between the two barriers, to the left of the first barrier and to the right of the second one. For each barrier we can use the results given above. The result for the transmission and reflection coefficients, in matrix form, reads

$$
\begin{pmatrix}
    a & b \\
    d & c
\end{pmatrix}
$$

Figure 4.4: Contour plot of the transmission through a double barrier for different magnetic fields with $W = 50$ nm, $W_s = 100$ nm, and $V = 100$ meV.

$\begin{pmatrix}
    1 \\
    r
\end{pmatrix} = M_L M_{W_s} M_R \begin{pmatrix}
    t \\
    0
\end{pmatrix} = M_D \begin{pmatrix}
    t \\
    0
\end{pmatrix}, \quad (4.9)$

here $M_L, M_R$ and $M_{W_s}$ are the transfer matrices to the left of the first barrier, to the right of the second barrier, and between the barriers, respectively. The element $M_{11}$ of the transfer matrix for a single barrier in polar coordinates is

$$
M_{11} = m_{11}e^{i\chi}, \quad (4.10)
$$

where

$$
m_{11} = \cos^2(\kappa W) + \left( \frac{1 - \cos \theta \sin \varphi}{\cos \theta \cos \varphi} \right)^2 \sin^2(\kappa W) \right)^{1/2}. \quad (4.11)
$$
4.2. POTENTIAL BARRIER AS A FABRY-PEROT INTERFEROMETER

Figure 4.5: The same as in Fig. 4.4 but for a double well with $V_1 = V_2 = -100$ meV.

The phase $\chi$ is given by

$$\chi = - \arctan \left[ \left( \frac{1 - s_0 s \sin \theta \sin \varphi}{s \cos \theta \cos \varphi} \right) \tan (\kappa W) \right] + k W, \quad (4.12)$$

where $s_i = \text{sgn}(E - V_i)$. Evaluating $M_{D11}$ we obtain

$$|M_{D11}|^2 = M_{L11} M_{R11} e^{-ik_x W} + M_{L12} M_{R21} e^{ik_x W}$$

$$= \left( |m_{11}|^2 - |M_{21}|^2 \right)^2 + 4|m_{11}|^2 |M_{21}|^2 \cos(k_x W_s - \chi), \quad (4.13)$$

where the matrix element $M_{21}$ of a single barrier is

$$M_{21} = \frac{1}{2 \cos \theta \cos \varphi} \left[ e^{i\theta} \cos(2\kappa a + \varphi) - i s_0 \frac{s_1}{s_1} \sin(2\kappa a) \right]$$

$$+ \left[ \frac{s_1}{s_1} \sin(2\kappa a) - s_0 e^{i\theta} \cos(2\kappa a - \varphi) \right]. \quad (4.14)$$

Then the transmission is given by

$$T_{tot}(E) = \frac{1}{|M_{11}|^2} = \frac{T_1^2}{T_1^2 + 4R_1 \cos^2(k_x W_s - \chi)}, \quad (4.15)$$
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where \( T_1 \) and \( R_1 = 1 - T_1 \) are the transmission and reflection coefficients of the single barrier (see Eq. (4.3)), respectively.

The minimum of the transmission occurs for \( k_x W_s - \chi = n\pi \) and is

\[
T_{\text{tot}}^{\text{min}} = \frac{T_1^2}{T_1^2 + 4R_1} = \frac{T_1^2}{(T_1 - 2)^2}. \tag{4.16}
\]

This is an increasing function of \( T_1 \) with a maximum value \( T_{\text{tot}}^{\text{min}} = 1 \) when \( T_1 = 1 \). Notice that here we cannot use the argument that the transmission through the single barrier is small since due to Klein tunneling \( T_1 = 1 \) for \( \kappa W = n\pi \) in which case Eq. (4.16) gives \( T_{\text{tot}}^{\text{min}} = 1 \). When the cosine in Eq. (4.16) vanishes the transmission approaches unity which occurs when \( T_{\text{tot}}^{\text{max}} = 1 \),

\[
k_x W_s - \chi = (2n + 1)\pi/2, \quad n = 0, 1, ..., \tag{4.17}
\]

where \( W_s \) is the distance between the two barriers. Then for a double barrier we have two conditions in order to have maximum transmission, namely,

\[
\kappa W = n\pi, \quad k_x W_s - \chi = (2n + 1)\pi/2, \quad n = 0, 1, ... \tag{4.18}
\]

Results for the transmission are shown in Fig. 4.4(a) for a double barrier. Notice that the numerical results are rather similar with those of a single barrier depicted in Fig. 4.2(a) for \( E > V \). The major difference is that the resonances are more pronounced and are not restricted to the cape region. Notice that for \( E < V \) the resonances for a single barrier have a concave \( E - k_y \) relation while for the resonant structure the behavior is convex (except near \( E \sim V/2 \)).

The above procedure can be repeated for symmetric double wells and the numerical results are shown in Fig. 4.5(a). As compared to the double barrier structure the resonances are very weak and the transmission is strongly enhanced and different from zero within the cone.

4.3 Fabry-Pérot resonances in the presence of a magnetic field

We start with a two-dimensional (2D) graphene sheet in the presence of a perpendicular magnetic field \( B(x) \) and a constant potential barrier of height \( V \) and width \( W \). An electron in this system is described by the Hamiltonian

\[
H = v_F \boldsymbol{\sigma} \cdot (\mathbf{p} + e\mathbf{A}(x)) + V. \tag{4.19}
\]
Then $\phi_1(x)$ and $\phi_2(x)$ obey the coupled first-order differential equations

$$-i\hbar v_F \left[ d/dx + (k_y + eA(x)/\hbar) \right] \phi_2 = \epsilon \phi_1, \quad (4.20a)$$

$$-i\hbar v_F \left[ d/dx - (k_y + eA(x)/\hbar) \right] \phi_1 = \epsilon \phi_2, \quad (4.20b)$$

where $\epsilon = E - V$. We now consider a homogeneous magnetic field $B_0$ and use the Landau gauge $A(x) = (0, B_0x, 0)$. Again we use the dimensionless variables $B(x) \to B_0B(x)$, $A(x) \to B_0\ell A(x)$, and set $\gamma = eB_0\ell^2/\hbar = \ell^2/\ell_B^2$, where $\ell_B$ is the magnetic length ($\ell_B = [\hbar/eB_0]^{1/2}$) with $\ell = 1 nm$. Then we can write $A(x) = \gamma x$. Further, by operating on Eqs. (4.20) with $-i[d/dx \pm (k_y + \gamma x)]$ we can decouple them. With $z = (2/\gamma)^{1/2}(k_y + \gamma x)$ the result is

$$[d^2/dz^2 - z^2/4 + p^\mp + 1/2] c_\mp = 0, \quad (4.21)$$

with $p^\mp = \epsilon^2/2\gamma \mp 1/2 - 1/2, c_\mp = \phi_1(z)$, and $c_+ = \phi_2(z)$. The solutions of Eq. (4.21) are the parabolic cylinder functions which can also be expressed as Weber functions [100]. The eigenfunctions $c_\pm$ are linear combinations of the linearly independent Weber functions $D(p, z)$ and $D(p, -z)$. Explicitly, with $\lambda = i\epsilon/(2\gamma)^{1/2}$ we have

$$\phi_1(z) = -A\lambda D(-\lambda^2 - 1, z) + B\lambda D(-\lambda^2 - 1, -z),$$

$$\phi_2(z) = AD(-\lambda^2, z) + BD(-\lambda^2, -z). \quad (4.22)$$

In the present chapter we are interested in learning how the tunnelling resonances are influenced by a magnetic field. We inject an electron beam with momentum $k = (k_x, k_y)$ towards the barrier and investigate the reflected and transmitted beams. If the magnetic field extends over the whole space, such a procedure cannot be used because electrons would be localized on cyclotron orbits. In a real experiment this is overcome by the diffusive motion of the electrons outside the barrier region. Therefore, for technical reasons, we limit the magnetic field to the barrier region, where transport is assumed to be ballistic when we deal with a single barrier, and to the resonant structure region when we deal with a multi-barrier structure. First we consider a single barrier, cf. Fig. 4.1(a). The solutions for the components $\phi_1(z)$ and $\phi_2(z)$ in the three spatial regions are

$$\phi_1(z) = \begin{cases} e^{ik_x x} + re^{-ik_x x} & x < 0 \\ \lambda [D(p - 1, -z) - cD(p - 1, z)] & 0 < x \leq W \\ te^{ik_x x} & x > W, \end{cases} \quad (4.23)$$

$$\phi_2(z) = \begin{cases} e^{ik_x x + i\phi} - re^{-ik_x x - i\phi} & x < 0 \\ cD(p, z) + dD(p, -z) & 0 < x \leq W \\ te^{ik_x x + i\phi} & x > W. \end{cases} \quad (4.24)$$
Here \( \lambda = i\varepsilon/\sqrt{2\gamma} \), \( p = \varepsilon^2/2\gamma \), \( \varepsilon = E - V \), \( k_x = (E^2 - k_y^2)^{1/2} \), \( k_x' = [E^2 - (k_y + \gamma W)^2]^{1/2} \), \( \tan \phi = k_y/k_x \), and \( \tan \varphi = (k_y + \gamma W)/k_x' \). To find the transfer matrix for this system we proceed as follows. For \( 0 < x < W \) the solution can be written as a combination of Weber functions. Matching the wave function at \( x = 0 \) and \( x = W \) gives the matrices

\[
N_1 = \begin{pmatrix} -\lambda D_{p-1}(z_0) & \lambda D_{p-1}(-z_0) \\ D_p(z_0) & D_p(-z_0) \end{pmatrix}, \\
N_2 = \begin{pmatrix} -\lambda D_{p-1}(z_W) & \lambda D_{p-1}(-z_W) \\ D_p(z_W) & D_p(-z_W) \end{pmatrix}.
\]

(4.25)

(4.26)

The transfer matrix \( M \) and the transmission \( T = 1/|M_{11}|^2 \) is determined by its element \( M_{11} \) given by

\[
M_{11} = \frac{[N_{11} + N_{12}e^{i\theta}e^{2ika} - i\theta] + [N_{21} + N_{22}e^{i\theta}]e^{2ika}}{2\cos \theta},
\]

(4.27)

with the matrix \( N \) given by \( N = N_1N_2^{-1} \). In a similar manner we obtain the results for a single well.

In the presence of a magnetic field the transmitted waves inside the barrier will

\[
\int_{\varphi_1}^{\varphi(x)} d\varphi \cos \varphi = \int_0^x dx \frac{\gamma}{E - V},
\]

(4.28)
and thus,
\[\sin \varphi_2(x) = \sin \varphi_1 + \frac{\gamma x}{E - V},\] (4.29)
from which we obtain a relation between the angle of incidence \(\theta_1\) and the angle of exit \(\varphi_2(W)\),
\[\sin \varphi_2(W) = \frac{E \sin \theta_1 + \gamma W}{E - V}.\] (4.30)
The critical angle \(\theta_c\) can be found by setting \(\varphi_2(W) = \pi/2\); it is
\[\sin \theta_c = \left(1 - \frac{V + \gamma W}{E}\right).\] (4.31)
and due to the inequality \(-1 < \sin \theta_c < 1\) we find
\[-\frac{V}{W} < \gamma < \frac{2E - V}{W}.\] (4.32)

Figure 4.7: Electron trajectories through a potential barrier in the presence of a magnetic field.

In the presence of a weak magnetic field the corresponding optical refractive index changes with the position \(x\) in the manner \(n(x) = 1 - \frac{V_{eff}(x)}{E}\). The function \(V_{eff}(x)\) plays the role of an effective potential. Let us consider
\[ V_{\text{eff}}(x) = V + g(x), \]
where \( V \) is the initial potential at zero magnetic field and \( g \) is a perturbation term due to the magnetic field. Using Eq. (4.29) we can evaluate \( g \) as,

\[ g(x) = \frac{\gamma(E - V)x}{(E - V) \sin \varphi_1 + \gamma x}. \tag{4.33} \]

For weak magnetic fields \( \gamma \) is small and the effective refractive index can be written as

\[ n(x) \approx 1 - \frac{V}{E} - \frac{\gamma x}{E \sin \varphi_1}. \tag{4.34} \]

The classical trajectory between 0 and \( W \) can be obtained from

\[ \frac{d^2 y}{dx^2} = \frac{1}{2\alpha^2} \frac{\partial n^2}{\partial x}, \tag{4.35} \]

with \( \alpha = (1 - V/E) \cos \varphi_1 \). If we neglect terms of order \( \gamma^2 \) the solution of Eq. (4.35) is

\[ y = -\frac{\gamma}{2(E - V) \sin \varphi_1 \cos^2 \varphi_1} x^2 + x \tan \varphi_1. \tag{4.36} \]

Using the same procedure as in Sec. 4.2 we obtain the classical optical path

\[ \Delta L \approx 2 \left(1 - \frac{V}{E}\right) W \cos \phi - \frac{\gamma W^2}{E} \left[1 + 2 \frac{\sin^2 \varphi_1}{\sin \varphi_1 \cos \varphi_2}\right], \tag{4.37} \]

where the first term is the optical path at zero magnetic field (see Eq. (2.52)). As shown in Fig. 4.7(a) for \( E > V \) the optical path decreases with increasing magnetic field while in Fig. 4.7(b) for \( E < V \) it increases. For \( E < V \), \( \varphi_2 \) increases very fast with magnetic field and the probability for the electron to pass through the barrier diminishes quickly. As shown later in Fig. 4.10 for \( E < V \), the resonances weaken with increasing magnetic field and finally disappear.

For double barriers or wells we follow the same procedure. Because the analytical results become too unwieldy, in what follows we present only the numerical results. A contour plot of the transmission through a double barrier, for different magnetic fields, is shown in Figs. 4.4(a)-(d) and through a double well in Figs. 4.5(a)-(d). We see clearly that increasing the magnetic field leads to a shift \( \Delta k_y = -\gamma(2W + W_s)/2 \) (and correspondingly to an induced energy gap \( \Delta E / E_0 = 2|\Delta k_y| \)) of the transmission cone, a reduction in the number of resonances, and a shrinking of the region of perfect transmission.
4.4. Conductance

Selecting the wave vector components $k_x$ and $k_y$ is very difficult, although in principle possible experimentally using quantum point contacts. However, experimentally one usually measures the average transmission. Typically one measures the current $J$ which is proportional to a weighted integral of the transmission.
 CHAPTER 4. FABRY-PÉROT RESONANCES IN GRAPHENE MICROSTRUCTURES: INFLUENCE OF A MAGNETIC FIELD

Figure 4.9: Contour plot of the conductance of a single barrier vs Fermi energy $E_F$ and barrier width $W$ for $V = 100$ meV and $B = 0.3T$.

Figure 4.10: Conductance of a single barrier and a single well for different magnetic fields with $W = 100$ nm and $V = 100$ meV. The inset is a blow-up of the region near 100 meV.

$T(k_x, k_y)$. For the linear spectrum $E = \hbar v_F k$ the conductance $G$ is given by

$$G = G_0 \int T(E, \theta) f(1 - f)E dE \cos \theta d\theta,$$

(4.38)
where \( f \equiv f(E - E_F) \) is the Fermi-Dirac distribution function and \( E_F \) the Fermi level. Further, \( G_0 = \frac{2e^2L}{v_F h^2} \) and \( L \) is the width of the entire structure along the \( y \) axis (\( L \gg W \)). With the explicit form of \( f \) the conductance becomes

\[
G(E_F) = G_0 \int_{-\infty}^{+\infty} EdE \int_{-\pi/2}^{\pi/2} T(E, \theta) \\
\times (\beta/4) \cosh^{-2} \left( \frac{\beta(E - E_F)}{2} \right) \cos \theta d\theta.
\]

(4.39)

with \( \beta = 1/k_B T \) and \( k_B \) the Boltzmann constant. Here we will restrict ourselves to zero temperature. Then the conductance takes the simpler form

\[
G = G_0 \int_{-\pi/2}^{\pi/2} T(E_F, \theta) E_F \cos \theta d\theta.
\]

(4.40)

Here we consider only the conductance through the tunnelling barrier(s) and neglect the contribution from the region before and after the resonant structure. Therefore, we only need the transmission \( T(E, \theta) \) through the resonant structure where it is allowed to restrict the magnetic field to the region of the resonant barrier structure.

First we consider the conductance for transport through a single barrier. In order to show more clearly the resonances we plot in Fig. 4.8 the second energy derivative of the conductance as a function of the Fermi energy \( E_F \) and the width of a single barrier for \( E_F < V \) in (a) and \( E_F > V \) in (b). In both cases the
magnetic field is zero. The positions of the resonances are approximately given by the dashed curves

$$E_n = V \pm n\pi/W; \quad (4.41)$$

the $+$ $(-)$ sign is for $E_F > V$ ($E_F < V$). For $E_F < V/2$, that is, to the left of the vertical dashed line in Fig. 4.8(a), we notice two types of peaks that have a different energy dependence. One is given by Eq. (4.41) and the other by Eq. (4.7). The latter increases much faster upon increasing the energy and asymptotically reaches the line $E = V/2$ for $W \to \infty$ as we show separately in Fig. 4.8(c). The latter resonances occur only for $E < V/2$ and this implies that the transmission maxima are connected to the bound states in the barrier region as given by Eq. (4.7). With reference to Fig. 4.2(b) we see that all these maxima occur for $E < V/2$. 

Figure 4.12: (a) Contour plot of the derivative of the conductance of a p-n-p structure vs potential $V$ and magnetic field for $W = 100$ nm. (b) Conductance of the structure in (a) vs potential for different magnetic fields $B = 0, 50, 100, 150, 200$ mT.
From the Bohr-Sommerfeld quantization condition we have [90, 101]

\[
\int_{x_-}^{x_+} p_x(x)dx = (n + 1/2 - \zeta)\pi\hbar
\]  

(4.42)

with

\[
p_x(x) = \left[ (E - V)^2 - (k_y + \gamma x)^2 \right]^{1/2},
\]

(4.43)

where \(x_-\) and \(x_+\) are the turning points, \(x_\pm = -k_y/\gamma \pm \varepsilon/\gamma\), \(\varepsilon = E - V\), and \(\zeta\) the Berry phase contribution which is 1/2 for Dirac fermions [102]. The integral
over \( x \) can be carried out. The result is
\[
I = \int_0^W p_x(x) dx = \frac{\varepsilon^2}{2\gamma} \left[ y[1 - y^2]^{1/2} + \arcsin y \right]_0^W \quad (4.44)
\]
with \( y = (k_y + \gamma x)/\varepsilon \). The transmission probability is symmetric about \( k_y = -q_0 = -\gamma W/2 \) and thus we find
\[
I = \left( \frac{\varepsilon}{\gamma} \right) \left[ q_0[1 - q_0^2]^{1/2} + \arcsin(q_0) \right]. \quad (4.45)
\]
For weak magnetic fields (\( \gamma \to 0 \)), the integral in Eq. (4.45) can be simplified to
\[
I \approx \int_0^W \left[ \kappa^2 - 2k_y\gamma x \right]^{1/2} dx. \quad (4.46)
\]
This gives
\[
\varepsilon_n \approx \pm \left[ \frac{n\pi}{2W} + \left( \frac{n\pi}{2W} \right)^2 + \left( \frac{\gamma W}{2} \right)^2 \right]^{1/2}. \quad (4.47)
\]
For \( \gamma = 0 \) Eq. (4.47) is exactly the same as Eq. (4.4) with \( k_y = 0 \). The difference between the spectrum with and without magnetic field is
\[
\Delta \varepsilon_n = \varepsilon_n^{B \neq 0} - \varepsilon_n^{B = 0}. \quad (4.48)
\]
4.4. CONDUCTANCE

Now we consider two different cases:

1) For $E < V$ we have

$$\Delta \varepsilon_n = n\pi/2W - \left[\left(\frac{n\pi}{2W}\right)^2 + \left(\frac{\gamma L}{2}\right)^2\right]^{1/2},$$

(4.49)

while for $\gamma = 0$ we easily obtain $\Delta \varepsilon_n = 0$. Because of $\Delta \varepsilon_n < 0$ we have $\varepsilon_n^{B \neq 0} < \varepsilon_n^{B = 0}$. This means that the resonance energies in the presence of a magnetic field shift below those for zero magnetic field. For the resonance energies in the range $0 < E < V$ we have also another limitation which comes from the energy gap opening through the magnetic field, $E_{\text{gap}} = \gamma W/2$. The resonance energies in the presence of a magnetic field can be reduced until the energy value becomes equal to $E_{\text{gap}}$ or simply $E_{\text{gap}} = \varepsilon_n^{B \neq 0}$. From this relation we can also find the number of resonances $n$ and the width $W$ after which the conductance drops to zero, see Fig. 4.9 for $0 < E < V$.

2) For $E > V$ we have

$$\Delta \varepsilon_n = -n\pi/2W + \left[\left(\frac{n\pi}{2W}\right)^2 + \left(\frac{\gamma L}{2}\right)^2\right]^{1/2}.$$

(4.50)

This means that the position of the resonances in the presence of magnetic field are shifted to higher energy or $\varepsilon_n^{B \neq 0} > \varepsilon_n^{B = 0}$, see Fig. 4.9 for $E > V$.

The conductance of a single barrier and that of a single well are shown in Fig. 4.10 for different magnetic fields $B$, the former to the right of the point $E_F = 0$ and the latter to its left. It is apparent from Fig. 4.10 that the conductance decreases with increasing magnetic field. We also see that there is a special point $E_F \approx V$ in the former where the conductance is almost insensitive to the value of the field $B$ and the inset makes that clear. This can be understood as follows. For $E_F \to V$ and $k_y \to \epsilon \to 0$ Eq. (4.3) shows that the transmission probability near the top of the barrier is

$$T \approx 1/\cosh^2(k_yW),$$

(4.51)

as previously obtained in Refs. [103] and [40] in the absence of a magnetic field. The corresponding conductance is,

$$G = \frac{4e^2}{v_F h^2} \frac{L}{W} \tanh(VW).$$

(4.52)

To see the dependence of the conductance on magnetic field more clearly, we show a contour plot of its logarithm in Fig. 4.11 for a single barrier. We notice that for $E_F > V$ the energy of the different resonances increase with $B$ whereas for $E_F < V$ they decrease. This opposite behavior can be understood as follows. In the limiting case $\gamma W \ll p^2$, that is, for $B \to 0$, to a first approximation the resonant energies are

$$E - E_n \sim \pm \gamma/2N,$$

(4.53)
Figure 4.15: Conductance of three asymmetric structures as shown in the inset with $W = 50$ nm and separation $W_s = 50$ nm. (a) $V_2 = 2V_1 = 200$ meV, (b) $V_3 = 3V_1$, $V_2 = 2V_1$ and $V_1 = 100$ meV, (c) $V_4 = 4V_1$, $V_3 = 3V_1$, $V_2 = 2V_1$, and $V_1 = 100$ meV.

Figure 4.16: Conductance of a double well for different magnetic fields with well width $W = 50$ nm, separation $W_s = 50$ nm, and $V_1 = V_2 = -100$ meV.

with $N = (n + 1/2)\pi/W$; the $+$ (−) sign is for $E > V$ ($E < V$) and $E_n$ is given by Eq. (4.41). Accordingly, these energies, as a function of the magnetic field, for $E_F > V$ have the opposite behavior compared to those for $E_F < V$. A contour
4.4. CONDUCTANCE

Figure 4.17: Conductance of the barriers shown in the inset for two different magnetic fields with $W = 100$ nm and $V = 100$ meV.

plot of the first derivative of the conductance of a p-n-p structure is shown in Fig. 4.12(a). The resonances in the conductance for several magnetic fields are shown in Fig. 4.12(b) where we plot the conductance of the p-n-p structure as a function of the potential height for fixed Fermi energy. The results are in good agreement with the experimental ones [91].

For $E_F \approx V$ the conductance for $B = 0$ exhibits a local minimum which is a signature of Klein tunneling. Notice that for $E_F < 0$ we have holes impinging on a quantum well and the conductance is similar to that for $E_F > V$. These resonances for 'normal' electrons are known as the Ramsauer effect. We found that they become more pronounced with increasing magnetic field. In the presence of a weak magnetic field, such that $\gamma W \ll V$ holds, the solution inside the barrier can be written as

$$
\Psi_{in}(x) = \begin{pmatrix}
A \exp \left[-(k_y - \gamma x)^2/(2\gamma)\right] \\
B \exp \left[-(k_y + \gamma x)^2/(2\gamma)\right]
\end{pmatrix}.
$$

(4.54)

Matching the solutions at $x = 0$ and $x = W$ gives

$$
\begin{cases}
1 + r = A \exp \left[-k_y^2/(2\gamma)\right] \\
re^{i\phi} - re^{-i\phi} = B \exp \left[-k_y^2/(2\gamma)\right]
\end{cases}
$$

(4.55)

and

$$
\begin{cases}
t e^{ik_y W} = A \exp \left[-(k_y - \gamma W)^2/(2\gamma)\right] \\
t e^{ik_y W + i\varphi} = B \exp \left[-(k_y + \gamma W)^2/(2\gamma)\right].
\end{cases}
$$

(4.56)
Then the transmission probability reduces to

$$T = \frac{4 \cos \varphi \cos \phi \exp(k_y^2/\gamma)}{S_+^2 + S_-^2 + 2S_+ S_- \cos(\phi + \varphi)}. \quad (4.57)$$

with $S_{\pm} = \exp[(k_y \pm \gamma W)^2/2\gamma]$. For $E \approx V$ and $\gamma W \ll V$ the transmission probability reduces to

$$T \approx \frac{e^{-\gamma W^2}}{\cosh^2(k_y W)}. \quad (4.58)$$

The corresponding conductance is

$$G = \frac{4e^2}{v_F \hbar^2} \frac{L}{W} \tanh(VW)e^{-\gamma W^2}. \quad (4.59)$$

Similar to the single-barrier case, in we show a contour plot of the logarithm of the conductance for a symmetric double barrier in Fig. 4.13(a) and an asymmetric one in Fig. 4.13(b). One feature common in both panels is the reduction of the conductance upon increasing $B$ and secondly an additional region in panel (b), centered around $E_F = 150$ meV, in which $G$ is significantly different from zero. We can see these features more clearly in the conductance $G$, shown in Fig. 4.14, for the symmetric double barrier (top panel) and the asymmetric one (bottom panel) for three values of $B$. For clarity the results for the symmetric case are shifted up by $0.15$. The first feature can be understood as follows. For $B = 0$ the wave vector to the left and right of the barrier is the same. This is not the case when $B$ is present because the wave vector component $k_y$ is shifted by $\gamma W$ (see Fig. 4.4). Then the green region in Fig. 4.1(c) will shrink and so will the transmission and the conductance. The second feature, in the bottom panel, centered around $E_F = 150$ meV in which $G$ is significantly different from zero, can be understood as follows. When the barrier heights $V_1$ and $V_2$ are equal, there is only one region, a rhombus, where tunneling involving real wave vectors is allowed. If these heights are different, then we have two such regions, one for each barrier. This is more clearly illustrated in Figs. 4.15(a)-(c), where we show, respectively, the conductance of two, three, and four asymmetric barriers shown at the bottom right of each panel. The other insets show pictorially these different transmission regions that are similar to that in Fig. 4.1. The vertical arrows pointing down in Fig. 4.15 and the corresponding parallel ones in the insets point to the same energies involved. Results to the right of the vertical arrows in the figure correspond to energies above the parallel arrows in the insets.

For completeness in Fig. 4.16 we show the conductance of a double, symmetric well (upper panel) and of an asymmetric one (lower panel) for positive energies.
(\(E_F > 0\)) with \(W = 50\) nm, separation \(W_s = 50\) nm, \(V_1 = V_2 = -100\) meV.
For clarity the results for the symmetric case are shifted up by 0.3. Had we plotted the results for \(E_F < 0\), the picture would be the same as Fig. 4.14. However, as expected for \(E_F > 0\), there is not much difference between the results of the two panels.

One may wonder how the results given above change if we don’t have abrupt interfaces of the rectangular barriers but instead consider, e.g., barriers or wells with smooth interfaces. We consider two such barriers, together with a square one, shown in the insets of Fig. 4.17. The second one is described by the semi-elliptic profile
\[
V(x) = \frac{2V}{W}[W^2/4 - (x - W/2)^2]^{1/2},
\]
and the third by the gaussian profile
\[
V(x) = V \exp[-(2\pi/W^2)(x - W/2)^2],
\]
where \(W\) is chosen such that the integral \(\int V(x)dx\) has the same value for all three potential barriers.

To evaluate the transmission for such shapes we subdivide their spatial extent or width in several square barriers of different height and for each of them we use the results of Sec. 4.3. Figure 4.17 contrasts the results of these shapes with those for a square barrier of height \(V\) for zero field in the lower panel and \(B = 5\) T in the upper one, which is shifted up by 0.15 for clarity. As can be seen, the results are qualitatively similar but the conductance for a square barrier is a bit larger when \(E_F < V\) and has a less pronounced peak structure. The resonant structure on the other hand is quantitatively different for the three cases as expected but qualitatively there are clear similarities.

### 4.5 Concluding remarks

We evaluated the transmission and conductance through single and double potential barriers and wells in the absence or presence of a magnetic field. We also considered different shapes of barriers as well as a few barriers with different potential heights. We placed the emphasis on the influence of these factors on the Fabry-Pérot resonances, that is, we studied them as Fabry-Pérot interferometers.

We obtained the energies for which the tunnelling probability is maximum for single and double barriers. The maxima in the transmission are connected with bound states, for energy smaller than \(V/2\), at \(E = \pm k_y\).

When a magnetic field is applied the cyclotron motion leads to a decrease in the transmission and consequently in the conductance. The magnetic field dependence...
of the position of the resonances is very different from the non-relativistic electron case: 1) their shift in energy is linear in magnetic field, and 2) for $E < V$ they decrease with the field, while for $E > V$ they increase.

For a single barrier we showed that the resonances in the transmission are reflected in those of the conductance. Extra resonances are found for $E_F < V/2$ which result from the connection between the maxima in the transmission and the bound states. For the special value $E_F = V$ we found that the conductance remains the same upon increasing the magnetic field and is given approximately by

$$G = \left( \frac{4e^2}{v_F h^2} \right) \left( \frac{L}{W} \right) \tanh \left( \frac{VW}{2} \right).$$

We showed that using asymmetric barriers, with unequal heights, we can create several different transmission or conductance regions in energy space involving only real wave vectors whereas for symmetric barriers with equal heights, there is only one such region.

We also evaluated the conductance of single barriers with smooth interfaces. We found that the oscillatory structure of the conductance becomes somewhat more pronounced but remains qualitatively the same as that of square barriers.
We evaluate the transmission through magnetic barriers in graphene-based nanostructures. Several particular cases are considered: a magnetic step, single and double barriers, and δ-function barriers. A separate class of magnetic barrier structures are those with inhomogeneous magnetic field profiles, such that the average magnetic field vanishes, that can be realized by nanostructured ferromagnetic stripes placed on top of the graphene layer. Quantum bound states that are localized near or in the barrier are predicted for a magnetic step and some structures with finite-width barriers but none for δ-function barriers. When a bound state is localized close to the barrier edge it has a non zero velocity parallel to this edge. The transmission depends strongly on the direction of the incident electron or hole wave vector and gives the possibility to construct a direction-dependent wave vector filter. In general, the resonant structure of the transmission is significantly more pronounced for (Dirac) electrons with "linear" spectrum than for the usual electrons with a "parabolic" spectrum.

5.1 Introduction

To circumvent the Klein tunneling and produce confined graphene-based structures, pertinent, e.g., to quantum computing and the design of devices in general, various schemes have been proposed: single-layer graphene strips [101,104], gated nanoribbons [105], gated and/or doped bilayers [106], etc. Another approach exploits the inherently two-dimensional (2D) motion through magnetic barriers initiated in Ref. [33] and recently applied to graphene, with a single magnetic barrier,

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in Ref. [57] and double barrier in Ref. [60]. In this chapter, using a considerable experience we acquired on motion through inhomogeneous magnetic fields [54] \(B\), we build on and significantly extend the latter approach by considering double and multiple magnetic barriers, \(\delta\)-function barriers, and barriers with a magnetic field profile in which \(B\) is reversed once or a few times within the same structure. The latter magnetic profile can be realized by ferromagnetic stripes [33] put on top of the graphene layer. Recently [50], edge states were studied in graphene in a nonuniform magnetic field.

### 5.2 Basic Formalism

#### 5.2.1 Homogenous magnetic field

An electron in a single graphene layer, in the presence of perpendicular magnetic field \(B(x)\), that may vary along the \(x\) direction is described by the Hamiltonian

\[
H_0 = v_F \sigma \cdot (p + eA(x)),
\]

where \(p\) is the momentum operator, \(v_F\) the Fermi velocity, and \(A(x)\) the vector potential. Here we first present results for a homogeneous magnetic field \(B_0\), with \(A(x) = (0, B_0 x, 0)\), and will contrast them later with those for inhomogenous magnetic fields. To simplify the notation we introduce the dimensionless units:

\[
\ell_B = \sqrt{\frac{\hbar}{e B_0}}, B(x) \rightarrow B_0 B(x), A(x) \rightarrow B_0 \ell_B A(x), t \rightarrow t \ell_B/v_F, r \rightarrow \ell_B r, v \rightarrow v_F v, E \rightarrow E_0 E, E_0 = \frac{\hbar v_F}{\ell_B}.
\]

In these units Eq. (5.1) is written explicitly as

\[
H = -i \begin{pmatrix} 0 & \partial_x - i \partial_y + x \\ \partial_x + i \partial_y - x & 0 \end{pmatrix}.
\]

Then the equation \(H \Psi(x, y) = E \Psi(x, y)\) admits solutions

\[
\Psi(x, y) = \begin{pmatrix} \psi_I(x, y) \\ \psi_{II}(x, y) \end{pmatrix},
\]

with \(\psi_I(x, y), \psi_{II}(x, y)\) obeying the coupled equations

\[
\begin{align*}
&i \left[ \partial/\partial x - i \partial/\partial y + x \right] \psi_{II} + E \psi_I = 0, \\
&i \left[ \partial/\partial x + i \partial/\partial y - x \right] \psi_I + E \psi_{II} = 0.
\end{align*}
\]

Due to the translational invariance along the \(y\) direction we assume solutions of the form \(\Psi(x, y) = \exp(ik_y y)(a(x), b(x))^T, T\) denoting the transpose of the row vector. Then Eqs. (5.37)a and (5.37)b take the form

\[
\begin{align*}
-i \left[ d/dx + (k_y + x) \right] b &= E a, \\
-i \left[ d/dx - (k_y + x) \right] a &= E b.
\end{align*}
\]
5.3. MAGNETIC FIELD STEP

Operating on Eqs. (5.5) with $-i(d/dx - (k_y + x))$ gives

$$\left[ d^2/dx^2 - (k_y + x)^2 \mp 1 + E^2 \right] c_\pm = 0, \quad (5.6)$$

where $c_- = a$ and $c_+ = b$. The solution of Eq. (5.6) are the well-known Hermite polynomials $H(x)$. For $c_- = a$ the wave function is $a(x) = \exp(-z^2/4)H_{E^2/2-1}(x + k_y)$ and the energy spectrum

$$E_n = \pm \sqrt{2(n+1)}. \quad (5.7)$$

Repeating this procedure for $c_+ = b$ gives $b(x) = \exp(-z^2/4)H_{E^2/2}(x + k_y)$ with spectrum

$$E_n = \pm \sqrt{2n}. \quad (5.8)$$

Notice the difference of these spectra from the one for the usual electrons $E_n = \hbar \omega_c(n + 1/2)$. The solution of Eq. (5.6) can also be written as a linear combination of the Weber functions $D_p(z)$ and $D_p-1(z)$ with $z = \sqrt{2}(x + k_y)$; as such it is more suitable for the case of inhomogeneous magnetic fields and will be used in Secs. III and IV.

5.2.2 Conductance

We will also calculate the conductance $G$ for various magnetic barrier structures by introducing it as the electron flow averaged over half the Fermi surface [33]

$$G = G_0 \int_{-\pi/2}^{\pi/2} T(E_F, E_F \sin \phi) \cos \phi \, d\phi. \quad (5.9)$$

Here $\phi$ is the angle of incidence relative to the $x$ direction, and $G_0 = 2e^2E_F\ell/\pi h$. For electrons with parabolic spectrum $E_F \sin \phi$ should be replaced by $\sqrt{E_F \sin \phi}$ and $G_0 = e^2m_F\ell/\hbar^2$, where $\ell$ is the length of the structure along the $y$ direction, and $v_F$ the Fermi velocity. $T(x, y)$ is the transmission through the studied structure.

5.3 Magnetic field step

5.3.1 General case

We consider a region $x < 0$, in which there is no magnetic field followed by one $x > 0$ in which there is a constant magnetic field $B$. This is formally described by

$$B(x) = B\Theta(x), \quad (5.10)$$
and was previously studied in Ref. [57]. For completeness we repeat the essential steps to find bound states close to the magnetic field step. In Sec. II we obtained the electron wave function in a constant magnetic field for \( x > 0 \). We have to match this wave function with that of a free electron for \( x < 0 \).

For a free electron the term \(+x\) in Eqs. (5.5)a, (5.5)b is absent and the wave function components \( a \) and \( b \) obey

\[
Ea + i (d/dx + k_y) b = 0, \tag{5.11a}
\]
\[
i (d/dx - k_y) a + Eb = 0. \tag{5.11b}
\]

Assuming exponential solutions \( a, b \sim e^{ik_x x} \) Eqs. (5.11)a and (5.11)b become two linear algebraic equations. Equating to zero the determinant of their coefficients gives

\[
E^2 = k_x^2 + k_y^2, \tag{5.12}
\]

with \( k_x \pm ik_y = (k_x^2 + k_y^2)^{1/2} \exp(\pm i\varphi) = E \exp(\pm i\varphi) \). For \( E^2 - k_y^2 > 0 \) the general solution is

\[
a(x) = fe^{ik_x x} + ge^{-ik_x x}, \tag{5.13a}
\]
\[
b(x) = fe^{ik_x x + i\varphi} - ge^{-ik_x x - i\varphi}, \tag{5.13b}
\]

while for \( E^2 - k_y^2 < 0 \) the solution is

\[
a(x) = S_+ fe^{ik_x x} + S_- ge^{-ik_x x}, \tag{5.14a}
\]
\[
b(x) = fe^{ik_x x} + ge^{-ik_x x}, \tag{5.14b}
\]

with \( S_\pm = -i(\pm k_x + k_y)/E \).

To properly match the solution for \( x < 0 \) to that for \( x > 0 \) at the step, we write the solutions for \( x > 0 \) as a linear combination of Weber functions \( D_p(x) \) and \( D_{p-1}(x) \). With \( p = E^2/2 \) and \( z = \sqrt{2}(x + k_y) \) this gives

\[
b = C D_p(z), \tag{5.15a}
\]
\[
a = -iC(E/\sqrt{2}) D_{p-1}(z). \tag{5.15b}
\]

\( C \) is a constant. Then matching the wave functions at \( x = 0 \) gives

\[
f - CD_{p-1}(\sqrt{2}k_y) = 0, \tag{5.16}
\]
\[
S_+ f + iC(E/\sqrt{2}) D_p(\sqrt{2}k_y) = 0. \tag{5.17}
\]

Setting to zero the determinant of the coefficients gives the spectrum \( E \), as a function of \( k_y \), by solving

\[
(\sqrt{2}(k_x + k_y)/E) D_p(\sqrt{2}k_y) = ED_{p-1}(\sqrt{2}k_y). \tag{5.18}
\]
Numerical results are shown in Fig. 5.1(a) and are identical to those of Ref. [57](b), except for the $n = 0$ level ($E = 0$) which was absent in Ref. [57]. Note that we have an infinite number of bound states labeled by the Landau level index $n$ in the $B > 0$ region. For $k_y \ll -1/\ell_B$ the center of the electron orbit $<x>$ is located deep in the magnetic region ($B > 0$) and the electron feels a homogeneous magnetic field. Then the bound state corresponds to the Landau level with energy $E = \pm \sqrt{2n}$. On the other hand, for $k_y \ell_B \rightarrow 0$ the spectrum approaches the free-electron spectrum in graphene, shown by the dashed orange line, since the center of the orbit comes closer and closer to the $B = 0$ region. This corresponds to the standard electron case discussed in Ref. [33] with the line $E = \pm \hbar v_F k_y$ replaced by the free-electron parabola.

### 5.3.2 Zero energy problem

The case $E = 0$ cannot be treated as outlined above and therefore was missed in Ref. [33]. This solution is also absent in the previous case of parabolic energy spectrum [54]. We assume $E = 0$ in Eqs. 5.37(a) and 5.37(b) and check if a bound state exists. Integrating these first-order differential equations gives

$$a = C_1 e^{(x+k_y)^2/2}, \quad b = C_2 e^{-(x+k_y)^2/2}. \quad (5.19a)$$

The solution for $b$ is acceptable: it vanishes for $x \rightarrow +\infty$, and consequently it is the wave function of a bound state. The solution for $a$ is not acceptable as it is not confined and therefore $C_1 = 0$. For $x > 0$ the resulting eigenfunction corresponding to the zero Landau level reads

$$\Psi = e^{ik_y y} e^{-(x+k_y)^2/2} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (5.20)$$

and the corresponding eigenvalue is $E = 0$.

Let us consider the $x < 0$ region where $B = 0$. The spectrum of a free electron is continuous with a peculiar point $E = 0$ also called the Dirac point. This becomes important when we construct bound-state eigenfunctions in magnetic-barrier structures. That is why we consider this eigenfunction in more detail below. Inserting $E = 0$ and $a, b \propto e^{ik_x x}$ in Eqs. 5.11(a)-5.11(b) we obtain

$$(k_x - ik_y) b = 0, \quad (5.21a)$$

$$(k_x + ik_y) a = 0. \quad (5.21b)$$

A homogeneous wave function is obtained only if the momentum is zero, that is, only for $k_x = k_y = 0$. Then the wave function components can have any value. However, if we are looking for a wave function only in some part of the
CHAPTER 5. DIRECTION-DEPENDENT TUNNELING

Figure 5.1: (a) Bound states energy spectrum vs the wave vector component ($k_y$) parallel to the magnetic step. The orange dashed line is the free-electron spectrum $E = \pm \hbar v_F k_y$. The upper inset shows a zoom of the $n = 1$ state near $E = k_y \hbar v_F$. The lower inset shows the magnetic field and vector potential profiles. (b) Wave function $b(x)$ for the $E = 0$ level for different values of the momentum $k_y$.

In the $xy$ plane, say in the region $x < 0$, one more solution is possible, namely one for
5.4. SIMPLE BARRIER STRUCTURES

\( a = 0, \ b \neq 0 \). Then Eq. (5.21)a gives \( k_x = i k_y \). Thus, for \( k_y < 0 \) we have

\[
\Psi = e^{i k_y y} e^{i |k_y| x} \begin{pmatrix} 0 \\ 1 \end{pmatrix}.
\]  

(5.22)

This is exactly what we need for matching it with the function (5.20) in the magnetic field region (\( x > 0 \)). As Eqs. (5.20) and (5.48) have only a single \( b \) component, the boundary condition can be satisfied by just choosing a proper coefficient. Thus, we have a bound state with zero energy as long as the momentum \( k_y \) is negative. When \( k_y \) vanishes, \( k_x \) is not positive any more: this means that an electron can escape to \(-\infty \) and the bound state disappears. Numerical results for the wave function are given in Fig. 5.1(b) and show clearly the increased leakage of the electron wave function into the magnetic barrier region for \(-k_y \to 0\).

5.3.3 Electron velocity

The bound states discussed above are bound only in the direction perpendicular to the magnetic step, i. e., they are localized close to the step but the electron (or hole) may propagate along the magnetic step, i. e., along the \( y \) direction. Below we evaluate the average velocity along the magnetic step \( v_n(k_y) \). We operate on Eqs. (5a)-(5b), for \( x > 0 \), and on Eqs. (5.11)a-(5.11)b for \( x < 0 \), with \( \partial / \partial k_y \) and integrate over \( x \). The result is

\[
-ia^* b = a^* a \left( \partial E / \partial k_y \right),
\]

(5.23a)

\[
ib^* a = b^* b \left( \partial E / \partial k_y \right),
\]

(5.23b)

and gives

\[
v_n(k_y) = \partial E / \partial k_y = \int_{-\infty}^{+\infty} dx \ j_y(x),
\]

(5.24)

where \( j_y = -i (a^* b - b^* a) \). Numerical results for \( v_n(k_y) \) are shown in Fig. 5.2 for various bound states. Notice that the electron and hole bound states have opposite velocities and consequently the direction of their current flow is the same. At the \( k_y \) value for which the bound state disappears the carrier attains the Fermi velocity, i. e., the velocity of an unbound particle in graphene.

5.4 Simple barrier structures

5.4.1 Single barrier

We consider a magnetic barrier in the region \(-d/2 < x < d/2\) as shown in the inset of Fig. 5.4. For \( x < d/2 \), \(-d/2 < x < d/2\), and \( x > d/2 \) the Hamiltonian is given
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Figure 5.2: Average electron \((E > 0)\) and hole \((E < 0)\) velocities along the magnetic step. The different bound states are labeled by the Landau level index \(n\).

by Eq. (5.1) with the upper (lower) off-diagonal elements shifted, respectively, by \(-d/2\), \((d/2)\), \(x\), \((-x)\) and \(d/2\), \((-d/2)\). Proceeding as in Sec. 5.2.1 we obtain for \(x < d/2\)

\[
\left(\frac{d^2}{dx^2} - q_-^2 + E^2\right) c = 0,
\]

(5.25)

where \(q_- = k_y - d/2\) and \(c = a, b\). By setting \(k_x^2 = E^2 - q_-^2\) and \(\tan \phi_1 = q_-/k_x\)

the solution for \(\Psi\) is

\[
\Psi_1 = \begin{pmatrix}
e^{ik_x x} + re^{-ik_x x} \\
e^{ik_x x+i\phi_1} - re^{-ik_x x-i\phi_1}
\end{pmatrix}.
\]

(5.26)

For \(-d/2 < x < d/2\) we have again Eq. (5.6). The corresponding solution is a linear combination of Weber functions

\[
\Psi_2 = \begin{pmatrix}
C_1 D_{p-1}(z) + C_2 D_{p-1}(-z) \\
(i\sqrt{2}/E)[C_1 D_p(z) - C_2 D_p(-z)]
\end{pmatrix},
\]

(5.27)

where \(z = \sqrt{2}(x + k_y)\) and \(p = E^2/2\). Finally, for \(x > d/2\) we define \(\tan \phi_2 = q_+/k_2\), \(q_+ = k_y + d/2\), and \(k_x^2 = E^2 - q_+^2\). Then the wave function takes the form

\[
\Psi_3 = \begin{pmatrix}
t e^{ik'_x x} \\
t e^{ik'_x x+i\phi_2}
\end{pmatrix}.
\]

(5.28)
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Matching the solutions and the flux at $x = -d/2$ and $x = d/2$ gives the transmission probability $T$. Setting $\alpha_1 = e^{-ik_x d/2}$, $\alpha_2 = e^{ik_x d/2}$, $\alpha_3 = D(p - 1, \sqrt{2q_-})$, $\alpha_4 = D(p - 1, -\sqrt{2q_-})$, $\gamma_1 = (i\sqrt{2}/E)D(p, \sqrt{2q_-})$, $\gamma_2 = (i\sqrt{2}/E)D(p, -\sqrt{2q_-})$, $\omega_1 = D(p - 1, \sqrt{2q_+})$, $\omega_2 = D(p - 1, -\sqrt{2q_+})$, $\eta_1 = (i\sqrt{2}/E)D(p, \sqrt{2q_+})$, $\eta_2 = (i\sqrt{2}/E)D(p, -\sqrt{2q_+})$, $\gamma_3 = e^{ik_x d/2}$, the result for $t$ is

$$t = \frac{2(\eta_2 \omega_1 + \eta_1 \omega_2) \alpha_1 \cos \phi_1}{\gamma_3 [f^+ g^+ - f^- g^-]}, \quad (5.29)$$

where $f^+ = \eta_2 + \omega_2 \exp i\phi_2$, $f^- = \eta_1 - \omega_1 \exp i\phi_2$, $g^+ = \gamma_1 + \alpha_3 \exp -i\phi_1$, and $g^- = \gamma_2 - \alpha_4 \exp -i\phi_1$. Then the transmission probability is given by,

$$T = (k_x'/k_x)|t|^2, \quad (5.30)$$

where the factor $k_x'/k_x$ is due to current conservation. From $k_x = |E^2 - (k_y - d/2)^2|^{1/2}$ we have the range of $k_y$ values $-E + d/2 \leq k_y \leq E + d/2$, and from $k_x' = |E^2 - (k_y + d/2)^2|^{1/2}$ the range $-E - d/2 \leq k_y \leq E - d/2$. This means that the acceptable range of $k_y$ values, for which the transmission result (5.30) holds, is

$$-E + d/2 \leq k_y \leq E - d/2. \quad (5.31)$$

Since $k_y = E \sin \phi_1 + d/2 = E \sin \phi_2 - d/2$, Eq. (5.31) gives the ranges for the angles $\phi_1$ and $\phi_2$, shown in Fig. 5.3,

$$-1 \leq \sin \phi_1 \leq 1 - d/E, \quad (5.32a)$$
$$-1 + d/E \leq \sin \phi_2 \leq 1. \quad (5.32b)$$

These ranges depend on $d/E$. The transmission is non zero only for $\phi_1$ and $\phi_2$ in these ranges and vanishes for $d \geq 2E$. For standard electrons Eq. (5.32) holds but with $d/E$ replaced by $d/(2E)^{1/2}$. A contour plot of the transmission coefficient is shown in Fig. 5.4 for a magnetic barrier with width $d = l_B$. Note that the transmission coefficient depends not only on the value of the momentum perpendicular to the magnetic barrier but also on the carrier momentum parallel to it. The boundary of the $T = 0$ region is well approximated by the classical result: $k_y = k_x^2/2d$.

The angular dependence of $T$ is made more clear in Fig. 5.5 where it is shown for different angles of incidence.

The spectrum of bound states is determined by

$$F^- (q_--) G^+ (-q_+) - F^+ (q_+) G^- (-q--) = 0, \quad (5.33)$$

with $F^\pm(z) = D_{p-1}(z) - (i\sqrt{2}/ES) D_p(z)$, $G^\pm(z) = D_{p-1}(z) + (i\sqrt{2}/ES) D_p(z)$, and $S_\pm = (i/E)[q_+ \mp (q_+ - E^2)^{1/2}]$. The dispersion relation (5.33) for $d = 5l_B$
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Figure 5.3: Schematics for the ranges of the possible angles of incidence $\phi_1$ and angles of exit $\phi_2$ for which electrons are able to propagate through the magnetic barrier.

Figure 5.4: Contour plot of the transmission $T$ through a magnetic barrier of width $d = l_B$. The inset shows the corresponding magnetic field and vector potential profiles.

is shown in Fig. 5.6 as a function of $k_y$. For $k_y > 0$ the bound states are localized near the $x \approx -d/2$ edge while for $k_y < 0$ they are localized near the $x \approx d/2$ edge.
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Figure 5.5: (a) Angular dependence of the transmission through a barrier of width \( d = l_B \) for different values of the electron energy. (b) As in (a) for an electron with energy \( E = 3.5 E_0 \) and different barrier widths.

There are seven bound states in Fig. 5.6 delimited by the free-electron spectrum \( E = \pm h v_F k_y \) (blue dashed lines). Notice that those for \( n \neq 0 \) have a nonzero velocity for energies different from the Landau levels \( E = \pm \sqrt{2n} E_0 \). The number of bound states \( n \) decreases with the width of the barrier but it is independent of its height. For \( d < 1.3 \ell_B \) only the \( E = 0 \) level is left as bound state.

5.4.2 Double barrier

We consider now a resonant tunneling structure, i.e., a double magnetic barrier shown in the inset of Fig. 5.7. The vector potential is given by

\[
A = \begin{cases} 
0, & x < -L/2 - d \\
1/d(x + (L/2 + d)), & -L/2 - d \leq x \leq -L/2 \\
1, & -L/2 < x < L/2 \\
1/d(x - (L/2 - d)), & L/2 \leq x \leq L/2 + d \\
2, & x > L/2 + d 
\end{cases}
\]  

Using Eq. (5.1) the procedure of Sec. 5.4.1 A is repeated in a straightforward manner and the transfer-matrix technique gives the transmission probability. The resulting expressions are very lengthy; here we will give only the numerical results.
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Figure 5.6: Energy spectrum $E$ of the bound states as a function of $k_y$ for a magnetic barrier of width $d = 5l_B$. Inset: magnetic field and vector potential profiles.

In Fig. 5.7 we show a contour plot of the transmission probability as a function of $k_x$ and $k_y$. As compared to a single barrier (see Fig. 5.4), the transmission exhibits a more pronounced structure. This is made clear in Fig. 5.8 upon comparing the inset with the main figure. The double barrier exhibits clear resonances that are absent in the single barrier. Notice that for electrons with a parabolic spectrum the resonances occur at different values of $k_x$ and are much weaker. The transmission depends strongly on the angle of incidence as made explicit in Fig. 5.9. In Fig. 5.9(a) we considered $d = l_B$ and $L = 2l_B$ and changed the energy while in Fig. 5.9(b) we fixed the energy $E = 3E_0$ and the distance between two barriers $L = 2l_B$ and changed the length of the barrier.

5.4.3 Structures with $< B > = 0$

In line with previous studies for standard electrons [54] and in search for more pronounced resonances, below we consider complex graphene structures with $< B > = 0$ and compare their transmission probability and conductance with those for standard electrons with a parabolic energy spectrum. In Fig. 5.10 we show a contour plot of the transmission probability for the complex structure shown in its inset. Such a magnetic field profile is a simple model for a strip magnetized per-
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Figure 5.7: Contour plot of the transmission $T$ through a double magnetic barrier with $d = l_B$ and $L = 3l_B$. The inset shows the magnetic field and vector potential profiles.

Figure 5.8: Transmission $T$ through a double magnetic barrier for Dirac electrons (dashed red curve) and standard electrons (solid black curve) with $d = l_B$, $L = 3l_B$. The upper inset shows the corresponding results for a single magnetic barrier.
Figure 5.9: (a) Angular dependence of the transmission through a double magnetic barrier for \( d = l_B, L = 2l_B \), and different electron energies. (b) As in (a) for \( E = 3E_0, L = 2l_B \), and different values of \( d \).

pendicular to the graphene [33] layer. Compared to the single-barrier structure of Fig. 5.4, the transmission is now symmetric with respect to \( k_y \rightarrow -k_y \) and exhibits a resonance behavior. When the strip is magnetized parallel to the layer but perpendicular to the magnetic strip, the magnetic field profile can be modeled by that given in the inset of Fig. 5.10. The corresponding contour plot of the transmission probability is shown in Fig. 5.10 for \( d = l_B \). Next we will use the above units to construct new resonant tunneling structures. In Fig. 5.12 we use the complex unit of Fig. 5.10 to build the structure with the field and corresponding vector potential profiles shown in its inset. The transmission exhibits strong resonances that are shown more clearly in Fig. 5.13. The resonances are more pronounced for Dirac electrons than for the usual electrons. Another resonant structure we can build with the unit of Fig. 5.11 is shown in the inset of Fig. 5.14. The corresponding contour plot of the transmission is shown in Fig. 5.14; it exhibits strong resonances along \( k_x \) and to a lesser extent along \( k_y \). A comparison with standard electrons is made in Fig. 5.15. Notice the much more pronounced resonances for massless Dirac electrons in Figs. 5.13 and 5.15 despite the similarity of Figs. 5.12 and 5.14 to Fig. 5 of Ref. [33]. In fact, the perfect transmission regions in Figs. 5.12 and 5.14 are much narrower than those in Fig. 5 of Ref. [33].
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Figure 5.10: Contour plot of the transmission $T$ through a complex magnetic barrier structure, shown in the inset, with $\langle B \rangle = 0$, well width $d = l_B$, and barrier width $L = 2l_B$.

Figure 5.11: Contour plot of the transmission $T$ through a complex magnetic barrier structure (see inset) with $\langle B \rangle = 0$ and barrier/well width $d = l_B$. 
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Figure 5.12: Contour plot of the transmission $T$ through the complex structure shown in the inset with $< B > = 0$, barrier width $d = l_B$, and well width $L = 3l_B$.

Figure 5.13: Transmission probability for a Dirac electron and a standard electron. The two-unit structure shown in the lower inset has $d = l_B$ and $L = 3l_B$. The upper inset shows the corresponding result through a single unit.
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Figure 5.14: Contour plot of the transmission through a two-unit resonant structure with $< B > = 0$, $d = 0.5l_B$, and $L = 3l_B$. The single unit is shown in Fig. 5.11.

Figure 5.15: Transmission probability for a Dirac electron and a standard electron. The structure shown in the upper inset has $d = l_B$ and $L = 3l_B$. The lower inset shows the corresponding transmission through a single unit.
Figure 5.16: A comparison of the conductance through two complex barrier structures, shown in the insets, for Dirac electrons \(E_0 = \hbar v_F / \ell_B\) and standard electrons \(E_0 = \hbar \omega_c\). The structures are characterized by \(d = 2\ell_B\) and \(L = 3\ell_B\).

We have also calculated the conductance \(G\) for these two structures, using Eq. (5.9), and compared it with that for standard electrons. In Figs. 5.16(a) and 5.16(b) we plot \(G\) as a function of the energy. The conductance is a quantity easier to measure than the momentum-dependent transmission coefficient. The resonances in \(G\), similar to those in the transmission, are more pronounced for Dirac electrons than for the usual electrons.
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5.4.4 Delta-function magnetic barriers

Analytical results for the transmission coefficient can be obtained if we consider \( \delta \)-function barriers [107]. Below we give the main results for single and double barriers.

For a single magnetic \( \delta \)-function barrier we have \( B(x) = B_0 \delta(x) \); the corresponding vector potential is \( A(x) = B_0 \theta(x) - \theta(-x)/2 \), where \( \theta(x) \) is the step function. For the chosen gauge \( k_y \) is a constant of motion and the wave function has the form \( \Psi(x,y) = e^{ik_y y} \psi(x) \).

In the dimensionless units of Sec. II the solution of the Schrödinger equation for a standard electron is

\[
\psi(x) = \begin{cases} 
  e^{ik_x x} + r e^{-ik_x x} & x < 0 \\
  t e^{ik'_x x} & x > 0.
\end{cases}
\tag{5.35}
\]

This results in the transmission probability

\[
T = |t|^2 \left( k'_x / k_x \right)
\tag{5.36}
\]

where \( t = 2k_x / (k'_x + k_x) \) and \( k'_x = \sqrt{2E + (k_y + 1)^2} \). Numerical results for \( T \) are shown in Fig. 5.17(a). For a Dirac electron the Hamiltonian is given by Eq. (5.2) with the upper (lower) off-diagonal elements shifted, respectively, by \( A(x) \) and \(-A(x)\). Looking again for solutions in the form of Eq. (5.3) we obtain

\[
-a \frac{d}{dx} (k_y + A(x)) b = Ea, \tag{5.37a}
\]
\[
-a \frac{d}{dx} (k_y + A(x)) a = Eb. \tag{5.37b}
\]

For \( x < 0 \) and \( E^2 - k_y^2 > 0 \) the solution for \( a \) and \( b \) is

\[
a(x) = e^{ik_x x} + re^{-ik_x x}, \quad b(x) = e^{ik_x x+i\phi} - re^{-ik_x x-i\phi},
\tag{5.38}
\]

where \( \tan \phi = k_y / k_x \). For \( x > 0 \) the result is

\[
a(x) = te^{ik'_x x}, \quad b(x) = te^{ik'_x x+i\theta}. \tag{5.39}
\]

With \( \tan \theta = (k_y + 1)/k'_x \) the transmission coefficient is

\[
t = 2 \cos(\phi) / (e^{i\theta} + e^{-i\phi}). \tag{5.40}
\]

where \( E = \pm \sqrt{k_x^2 + (k_y + 1)^2} \). Then the continuity of the wave function gives the transmission probability

\[
T = \left( k'_x / k_x \right) |t|^2. \tag{5.41}
\]
A contour plot of this transmission probability is shown in Fig. 5.17(b). Notice that Dirac electrons have a smaller window for $T \approx 1$ transmission as compared to the standard electrons. There are no qualitative differences between the results for a $\delta$-function barrier (Fig. 5.17(b)) and those for a barrier of finite width, (Fig. 5.4).

We know that a $\delta$-function potential well has one bound state. Let us investigate if a $\delta$-function magnetic barrier has any bound state. If it does, it’s expected to
occur for \( k_y^2 > E^2 \). For \( x < 0 \) the wave function is
\[
\psi(x) \sim e^{ik_y y} e^{ik_x x} \left( \frac{1}{(-i/E)(k_x - k_y^-)} \right),
\] (5.42)
while for \( x > 0 \) there is a constant vector potential; with \( k_y^\pm = k_y \pm 1/2 \) the wave function is
\[
\psi(x) \sim e^{ik_y y} e^{-k'_x x} \left( \frac{1}{(i/E)(k'_x + k_y^+)} \right),
\] (5.43)

Matching the wave functions at \( x = 0 \) we obtain
\[
[(k_x^+)^2 - E^2]^{1/2} + [(k_y^-)^2 - E^2]^{1/2} + 1 = 0;
\] (5.44)
this equation cannot be satisfied and therefore a magnetic \( \delta \)-function barrier does not have any bound states. We now consider the special case \( E = 0 \). For \( x < 0 \) Eqs. 5.5(a) and 5.5(b) give \( (d_- = b, d_+ = a) \)
\[
(k_x \mp ik_y^-)d_- = 0,
\] (5.45)
The wave function with \( a = 0, b \neq 0 \), is
\[
\Psi_I \sim e^{ik_y y} e^{-k_y x} \left( \begin{array}{c} 0 \\ 1 \end{array} \right).
\] (5.46)
For \( x < 0 \) Eq. (5.48) can be a solution if \( k_y^- < 0 \). In the region \( x > 0 \) Eqs. 5.37(a) and 5.37(b) become
\[
(k'_x \mp ik_y^+)d_+ = 0;
\] (5.47)
the corresponding wave function is
\[
\Psi_{II} \sim e^{ik_y y} e^{-k_y^+ x} \left( \begin{array}{c} 0 \\ 1 \end{array} \right).
\] (5.48)
In order to have a proper solution for \( x > 0 \) it is convenient to choose \( k_y^+ > 0 \). Thus we have a line of bound states with \( E = 0 \) and \(-1/2 < k_y < 1/2\).

For a resonant tunneling structure, consisting of two \( \delta \)-function magnetic barriers, we can combine the results for two single barriers and obtain the transmission through the structure. Solving \( H \Psi = E \Psi \) we obtain
\[
A(x, y) = \begin{cases} 
  e^{ik_x x + ik_y y} + re^{-ik_x x + ik_y y} & x < -L/2 \\
  ae^{ik'_x x + ik_y y} + be^{-ik'_x x + ik_y y} & |x| \leq L/2 \\
  te^{ik_x x + ik_y y} & x > L/2
\end{cases}
\] (5.49)
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Figure 5.18: Contour plot of the transmission probability through two opposite \( \delta \)-function barriers, see inset, with \( L = 4l_B \).

Figure 5.19: (a) The conductance through one \( \delta \)-function barrier with \( L = 4l_B \) for a Dirac electron (solid red curve) and a standard electron (dashed black curve) with \( E_0 = \hbar \omega_c \). (b) As in (a) but for two \( \delta \)-function barriers with the magnetic field in the same direction.

\[
B(x, y) = \begin{cases} 
  e^{ik_x x + ik_y y + i\phi} - re^{-ik_x x + ik_y y - i\phi} & x < -L/2 \\
  ae^{ik_x x + ik_y y + i\theta} - be^{-ik'_x x + ik_y y - i\theta} & |x| \leq L/2 \\
  te^{ik_x x + ik_y y + i\phi} & x > L/2 
\end{cases}
\]

Matching the solutions at \(-L/2\) and \(L/2\) gives

\[
t = \frac{2 \cos \phi \cos \theta e^{-ik_x L}}{e^{-ik_x L} \cos(\theta + \phi) + 1 + e^{ik_x L} \cos(\theta - \phi) + 1}.
\]
5.4. SIMPLE BARRIER STRUCTURES

Here \( k_x = [E^2 - (k_y)^2]^{1/2} \), \( k'_x = [E^2 - (k_y + 1)^2]^{1/2} \), \( \tan \phi = k_y/k_x \), and \( \tan \theta = (k_y+1)/k'_x \). A contour plot of the transmission probability, through two opposite \( \delta \)-function barriers, is shown in Fig. 5.18. The transmission exhibits a clear resonant behavior which has a qualitatively different \((k_y, k_x)\) dependence than that of the resonant structures shown in Figs. 5.18, 5.12, and 5.14. When we interchange the sign of the two barriers, i.e. \( B \rightarrow -B \), we obtain the same transmission with \( k_y \rightarrow -k_y \).

For two successive \( \delta \)-function barriers with the magnetic field in the same direction we obtain \((\theta_\pm = \theta \pm k'_x L)\)

\[
t = \frac{2 \cos \phi \cos \theta e^{-i(k_x+k'_x)L/2}}{e^{i\eta \cos (\theta_-)} + e^{-i\phi \cos (\theta_+)} - (1 + e^{i(\eta-\phi)})i \sin k'_x L}.
\]  

(5.52)

Here \( k''_x = [E^2 - (k_y + 2)^2]^{1/2} \) and \( \tan \eta = (k_y + 2)/k''_x \). A contour plot of

Figure 5.20: Contour plot of the transmission probability for two \( \delta \)-function barriers in the same direction with \( L = 4l_B \). The inset shows the magnetic field and vector potential profiles.

the transmission is shown in Fig. 5.20 and the conductance in Fig. 5.19(b). The transmission in Fig. 5.20 has some similarity with the finite-width barrier result shown in Fig. 5.7; the difference here is that resonances are more pronounced and their number is increased.
5.5 Conclusions

We evaluated the transmission through various magnetic barrier nanostructures based on graphene. In particular, we treated in detail a magnetic step, single and double regular or \( \delta \)-function barriers as well as complex structures with inhomogeneous magnetic field profiles but such that the average magnetic field vanishes.

We obtained bound states that are localized near the magnetic step or the edges of the regular barriers but not for \( \delta \)-function barriers. Our results agree with the limited ones, for a single barrier in Ref. [57] a) and a step in Ref. [57] b), but importantly they differ in the \( E = 0 \) bound state which was not obtained in Ref. [57]. In addition, we showed that the transmission exhibits a strong dependence on the direction of the incident electron or hole wave vector. In general, the resonant structure of the transmission is significantly more pronounced for Dirac electrons with linear spectrum than for those with a parabolic spectrum. Moreover, the transmission through the complex structures of Sec. V shows a much more pronounced resonances than that through single or double barriers. To our knowledge these results are new.

An important feature of the transmission results is their dependence on the angle of incidence as shown in several figures and highlighted in Ref. [57] for a single barrier: the transmission is finite only in a certain range of angles of incidence, shown for a single barrier schematically in Fig. 5.3 and more explicitly in Fig. 5.5. One can further modify the angular dependence of the transmission with double barriers, cf. Fig. 5.9. The main parameters that control this angular dependence are the width of the barriers/wells and the energy of the incident electrons.

A further aspect of our results for graphene-based nanostructures, involving electrons with a nearly linear spectrum, is their contrast with those for standard electrons characterized by a parabolic spectrum [33], see Figs. 5.8, 5.13, 5.15, 5.16, and 5.19. We saw a marked difference not only in the transmission but also in its average over half the Fermi surface, that is, the conductance given by Eq. (5.9), see Figs. 5.16 and 5.19. The resonant behavior, especially for double barriers, is significantly more pronounced for electrons with a nearly linear spectrum. The behavior of the conductance shown in Fig. 5.19, for a linear spectrum, is similar to that through a double barrier created by two ferromagnetic stripes placed above a graphene layer [62].
Tunneling, conductance, and wavevector filtering through magnetic barriers in bilayer graphene

Abstract. We evaluate the transmission and conductance through magnetic barrier structures in bilayer graphene. In particular we consider a magnetic step, single and double barriers, δ-function barriers, as well as barrier structures that have average magnetic field equal to zero. The transmission depends strongly on the direction of the incident electron or hole wave vector and gives the possibility to construct a direction-dependent wave vector filter. The results contrast sharply with previous results on single-layer graphene. In general, the angular range of perfect transmission becomes drastically wider and the gaps narrower. This perfect transmission range decreases with the number of barriers, the barrier width, and the magnetic field. Depending on the structure, a variety of transmission resonances occur that are reflected in the conductance through the structure.

6.1 Introduction

In contrast to carriers in single-layer graphene, those in bilayer graphene possess a quadratic spectrum near the K-points and show no Klein tunneling [32]. Adsorbates and/or gate potentials induce an energy gap due to the tunnel coupling between the layers that is more appropriate for certain applications, e. g., for improving the on/off ratio in carbon-based transistors. A recent review of the properties of graphene is given in Ref. [2]. In a previous chapter we studied the transmission through magnetic barrier structures and its angular confinement in single-layer graphene. In doing so we extended significantly earlier limited results [57] for a barrier and a step by considering double barriers, δ-function barriers, and barrier

*The results of this chapter were published as:
structures with inhomogeneous magnetic field profiles which have average magnetic field zero that can be realized using nanostructured ferromagnetic strips that are positioned above the graphene layer. We also contrasted the results for electrons with those obtained from the Schrödinger equation [33, 54, 107]. The aim of the present work is to extend our previous study on tunneling through various magnetic barrier structures to bilayer graphene (see Fig. 6.1 for the layout of the system) and critically contrast them with those for single-layer graphene [50, 57, 58, 60, 62]. As will be seen, the tunnel coupling between the layers significantly modifies some results and further supports bilayer graphene as a promising material for carbon-based devices.

### 6.2 Basic Formalism

#### 6.2.1 Homogenous magnetic field

Before we consider transport in the presence of inhomogeneous magnetic fields we present the energy levels and corresponding wavefunctions in a constant magnetic field. Consider a homogeneous magnetic field $B_0$ normal to the two-dimensional (2D) plane $(x, y)$ of bilayer graphene. To study transmission through one-dimen-

sional (1D) magnetic barriers we use the Landau gauge for the vector potential $\mathbf{A}(x) = (0, B_0 x, 0)$ and make the change $p \rightarrow p + eA$, where $p$ is the momentum operator. The one-electron Hamiltonian for a graphene bilayer is

$$
H = \begin{pmatrix}
V_1 & \Pi & t & 0 \\
\Pi^\dagger & V_1 & 0 & 0 \\
t & 0 & V_2 & \Pi^\dagger \\
0 & 0 & \Pi & V_2
\end{pmatrix},
$$

(6.1)
with $\Pi = v_F[p_x + i(p_y + eA)]$, where $v_F = 1 \times 10^6 m/s$ is the Fermi velocity, $V_1$ and $V_2$ are the potentials at the two layers and $t$ is the tunnel coupling between the layers, assumed to be constant. This Hamiltonian is valid near the Dirac point $K$ or $K'$. Thus scattering between the $K$ and $K'$ valleys is neglected. This scattering was shown [50] to be negligible for fields below $10^4 T$ in single-layer graphene; we expect this to be the case in bilayer graphene as well. It also neglects the real spin.

Energy is of the order of $10^4$ meV or $\lesssim$ layers, assumed to be constant. This Hamiltonian is valid near the Dirac point $K$. Thus scattering between the $K$ and $K'$ valleys is neglected. This scattering was shown [50] to be negligible for fields below $10^4 T$ in single-layer graphene; we expect this to be the case in bilayer graphene as well. It also neglects the real spin of the electrons. However, for the fields of interest here, $B_0 \leq 1 T$, the Zeeman energy is of the order of $10^{-1}$ meV, i.e., negligible compared to the Fermi energy $E_F \sim 10$ meV [12]. For more details as well as the neglect of trigonal warping, appropriate for high energies, see Ref. [35].

To simplify the notation we introduce the length scale $\ell_B = [\hbar/eB_0]^{1/2}$ and the energy scale $E_0 = \hbar v_F/\ell_B$. This allows us to define the following dimensionless quantities: $B(x) \to B_0 B(x)$, $A(x) \to B_0 \ell_B A(x)$, $r \to \ell_B r$, $v \to v_F v$, $E \to E_0 E$, $t \to E_0 t$. The Hamiltonian commutes with $p_y$ and therefore is a conserved quantity. This allows us to write $\Psi(x, y) = \Phi(x) \exp(ik_y y)$ and solve the equation $H\Psi(x, y) = E\Psi(x, y)$ for the wave function

$$
\Psi(x, y) = \begin{pmatrix}
\phi_\alpha(x) \\
\phi_b(x) \\
\phi_c(x) \\
\phi_d(x)
\end{pmatrix} e^{ik_y y}
$$

with $T$ denoting the transpose. Then the components of $\Psi(x, y)$ obey the following coupled differential equations

$$
\begin{align*}
-i(d/dx - (k_y + x))\phi_b + t'\phi_c &= (E - V_1)\phi_a, \\
-i(d/dx + (k_y + x))\phi_a &= (E - V_1)\phi_b, \\
-i(d/dx + (k_y + x))\phi_d + t'\phi_a &= (E - V_2)\phi_c, \\
-i(d/dx - (k_y + x))\phi_c &= (E - V_2)\phi_d.
\end{align*}
$$

Setting $V_0 = (V_1 + V_2)/2$, $\Delta V = V_1 - V_2$, $\delta = \Delta V/2$, and $\epsilon = E - V_0$, Eqs. (6.3) can be decoupled by eliminating the unknowns one at a time. The result for $\phi_a$ is

$$
[d^2/dz^2 - z^2/4 + \gamma_{\pm}/2] \phi_a = 0.
$$

where $\gamma_{\pm} = \epsilon^2 + \delta^2 \pm [(1 - 2\delta\epsilon)^2 + (\epsilon^2 - \delta^2)t^2]^{1/2}$ and $\sqrt{2}(x + k_y) = z$. The solutions of Eq. (6.4) can be written in terms of the Weber functions. For an asymptotically vanishing wave function for $z \to \infty$ we define $\phi_a(z) = e^{-z^2/4}g(z)$ and
substitute it in Eq. (6.4). For $\delta = 0$ and using standard power-series procedures we complete the solution and find the energy spectrum

$$
\epsilon_{n,\pm} = \pm \left[ 2n + 1 + \frac{t'^2}{2} \pm \left[ \frac{t'^4}{4} + (2n + 1)t'^2 + 1 \right]^{1/2} \right]^{1/2},
$$

(6.5)

where $n$ is an integer, the Landau-level index. Notice the similarity with the spectrum for single-layer graphene, $E_n = \pm \sqrt{2(n + 1)}$ or $E_n = \pm \sqrt{2n}$ and the difference from that for the usual electrons with parabolic energy momentum relation: $E_n = \hbar \omega_c (n + 1/2)$ consisting of equidistant Landau Levels. For $t \to 0$, Eq. (6.5) reduces to that of two uncoupled layers with spectrum $E_n = \pm \sqrt{2n + 1} \pm 1$. The spectrum for the first three lowest levels is shown in Fig. 6.2 as a function of the strength $t$ of the interlayer coupling for a constant magnetic field $B = 1$ T. The usual value $t = 400\text{meV}$ corresponds to $t' = 15$. Notice that varying $t'$ for fixed $t$ is equivalent to changing the magnetic field, because $E_0 \sim \sqrt{B}$. In the rest of the paper we fix $t = 400\text{meV}$.

The solution of Eq. (6.4) can be also written in terms of the well-known Hermite polynomials $H_n(x)$. However, this solution is not well suited for regions with discontinuities in the magnetic field that we study here. For this reason we will use Weber functions which are more appropriate. The various wave function compo-
6.2. BASIC FORMALISM

components, up to a normalization constant, are

\[ \Phi^{\pm}(z) \sim \begin{pmatrix} D(p^{\pm}, z) \\ (-i\sqrt{2}p^{\pm}/\epsilon)D(p^{\pm} - 1, z) \\ (\epsilon/t' - 2p^{\pm} / (t\epsilon))D(p^{\pm} z) \\ (i\sqrt{2}/\epsilon)(\epsilon/t' - 2p^{\pm} / (t\epsilon))D(p^{\pm} + 1, z) \end{pmatrix}, \]  

(6.6)

where \( p^{\pm} = (\gamma^{\pm} - 1)/2 \). In regions where the magnetic field is zero and for constant potentials \( V_1 \) and \( V_2 \) with \( \delta = 0 \) we introduce the right-moving solutions

\[ \Psi_{R}^{\epsilon, \pm}(x, y) = N^{\pm} \left[ \mp \epsilon, \pm k^{\pm}_x \pm ik_y, \epsilon, k^{\pm}_x + ik_y \right]^T f^+, \] 

(6.7)

and the left-moving ones \( (N^{\pm} = (4L_y\epsilon k^{\pm}_x)^{-1/2}) \)

\[ \Psi_{L}^{\epsilon, \pm}(x, y) = N^{\pm} \left[ \mp \epsilon, \pm k^{\pm}_x \pm ik_y, \epsilon, -k^{\pm}_x + ik_y \right]^T f^-, \] 

(6.8)

with \( f^{\pm} \equiv f(x, y) = e^{\pm i k^{\pm}_x x + i k_y y} \) and \( L_y \) the length of the structure along the \( y \) direction. The corresponding energy spectrum and wave vector are

\[ \epsilon = \mp t'/2 \pm \left[ t'^2/4 + K^{\pm} \right]^{1/2}, \] 

(6.9)

\[ k^{\pm}_x = \left[ \epsilon^2 - k^2_y \pm \epsilon t' \right]^{1/2}, \] 

(6.10)

where \( K^{\pm} = k^{2\pm}_x + k^2_y \). The normalization factor \( N^{\pm} \) is obtained from the requirement of unit current carried by each state in the positive or negative \( x \)-direction

\[ I = ev \int_{0}^{W} dy \Psi^\dagger \begin{pmatrix} \sigma_x & 0 \\ 0 & \sigma_x \end{pmatrix} \Psi. \] 

(6.11)

6.2.2 Conductance

We will also calculate the conductance \( G \) for various magnetic barrier structures by introducing it as the electron flow averaged over half the Fermi surface [33]. We evaluate \( G \) from the standard expression for the total current density \( J \), from left to right, given by

\[ J = -e \int_{0}^{\infty} dE \int_{-\pi/2}^{\pi/2} T(E, \phi) [f_l(E) - f_v(E)] v_x(E) \rho(E) E d\phi. \] 

(6.12)
Here $f_l(E) (f_r(E))$ is the Fermi-Dirac function on the left (right), $\rho(E)$ the density of states, and $T(E, \phi)$ the transmission as a function of the energy $E$ and the angle of incidence $\phi$ relative to the $x$ direction. In the linear transport regime and for low temperatures we can replace $f_l - f_r$ by a $\delta$ function and obtain the conductance

$$G = G_0 \int_{-\pi/2}^{\pi/2} T(E_F, E_F \sin \phi) \cos \phi \, d\phi,$$

(6.13)

with $G_0 = (2e^2/h)(L_y/\pi \hbar v_F)\left[ E_F^2 + tE_F \right]^{1/2}$ and $E_F$ the Fermi energy.

### 6.3 A magnetic field step, single and double barriers

#### 6.3.1 Magnetic field step

We consider a region $x < 0$, in which there is no magnetic field, followed by one $x > 0$ in which there is a constant magnetic field $B$. This is described by

$$B(x) = B_0 \Theta(x).$$

(6.14)

For $x < 0$ the solution is that of a free particle while for $x > 0$ the solution is a combination of the solutions for the homogenous magnetic field case, i.e., Eq. (6.6). The solution for $x < 0$ can be written as

$$\Psi_{+}^{\pm}(k_x, z^\pm) = e^{\pm i k_x x} \left[1, \mp \frac{i}{\epsilon}(\pm k_x^+ + k_y), \mp 1, \pm \frac{i}{\epsilon}(\pm k_x^- - k_y)\right]^T.$$  

(6.15)

and the full wave function is

$$\Psi^I = c_1 \Psi_{+}^{+} + c_2 \Psi_{-}^{+}.$$  

(6.16)

For $x > 0$ the result is

$$\Psi^{II} = c_3 \Phi^+(z) + c_4 \Phi^-(z),$$

(6.17)

with $z = \sqrt{2}(x + k_y)$ and $\Phi^\pm(z)$ given by Eq. (6.6). Matching the solutions at $x = 0$ gives the homogeneous set of algebraic equations in the matrix form

$$\begin{pmatrix}
1 & 1 & s^+ & s^- \\
1 & 1 & b^+ & b^- \\
a^+ & a^- & f^+ & f^- \\
e^+ & e^- & g^+ & g^-
\end{pmatrix}
\begin{pmatrix}
c_1 \\
c_2 \\
c_3 \\
c_4
\end{pmatrix} = 0.$$  

(6.18)
Here \( z^\pm = \frac{i}{E}(k_x^\pm + k_y), \) \( e^\pm = \frac{i}{E}(k_x^\pm - k_y) \alpha^\pm, s^\pm = D(p^\pm, \sqrt{2} k_y), \) \( f^\pm = \frac{E^\pm - 2p^\pm}{E} s^\pm, \) \( b^\pm = (i\sqrt{2} p^\pm / \epsilon) D((p^\pm - 1, \sqrt{2} k_y), \) \( g^\pm = (i\sqrt{2} / \epsilon)(\epsilon / t' - 2p^\pm / (t' \epsilon)) D(p^\pm + 1, \sqrt{2} k_y) \) and \( a^\pm = \epsilon / t' + (k_x^\pm^2 - k_y^2) / (\epsilon t'). \) The dispersion relation is obtained from the condition \( \det(M) = 0. \) As a function of \( k_y \) the spectrum is shown in Fig. 6.3(a). We contrast it with that for a single-layer in Fig. 6.3(b). Both spectra terminate at the corresponding free-electron results with the single-layer straight lines \( E = \hbar v_F k_y \) in (b) replaced by the parabolas \( E = \hbar v_F k_y \mp t'/2 \pm (t'^2/4 + k_y^2)^{1/2} \) in (a). Notice also how different the level spacing is between the two panels. For large negative \( k_y \) the particles, localized

![Figure 6.3](image_url)

**Figure 6.3:** Bound states energy spectrum vs wave vector component \( k_y \) parallel to the magnetic step. Panel (a) is for a bilayer step with \( t' = 15 \) and panel (b) for a magnetic step in single-layer graphene.

around \( x_0 = -k_y B \), are deep into the magnetic field region and their spectrum is that of the previously mentioned Landau levels. For \( k_y \) values close to the free-particle branch (dotted curves) the energy spectrum attains a dispersion (with the exception of the \( n = 0 \) or \( E = 0 \) level) implying that the states have a non zero velocity. Such states are confined in the \( x \) direction near the barrier edge (see Fig. 6.4) and move along it.
Figure 6.4: The electron probability density $|\Psi|^2 = |\phi_a|^2 + |\phi_b|^2 + |\phi_c|^2 + |\phi_d|^2$ of the $n = 1$ Landau level, in a magnetic step, for different values of $k_y$.

### 6.3.2 Single and double barrier

#### Energy spectrum

We consider a magnetic barrier of width $d$ shown in the inset of Fig. 6.5(a). The corresponding vector potential $A(x)$ is given by

$$A(x) = B_0 \begin{cases} 
-d/2 & x < -d/2 \\
 0 & -d/2 < x < d/2 \\
 d/2 & x > d/2 
\end{cases} . \quad (6.19)$$

In region I for $(x < -d/2)$ the solution can be written as

$$\Psi^I = c_1 \Psi^+_E k_x^+ + c_2 \Psi^+_E k_x^- , \quad (6.20)$$

in region II $(-d/2 < x < d/2)$ as

$$\Psi^{II} = f_1 \Phi^- (z) + f_2 \Phi^- (-z) + f_3 \Phi^+ (z) + f_4 \Phi^+ (-z) , \quad (6.21)$$

with $z = \sqrt{2}(k_y + x)$, and in region III $(x > d/2)$ as

$$\Psi^{III} = h_1 \Psi^-_E k_x^+ + h_2 \Psi^-_E k_x^- . \quad (6.22)$$

The continuity of the wave function at the edges of the barrier, $x = \pm d/2$, and current conservation give

$$\Psi^I_{k_x^+} (-d/2) = \Psi^{II} (-d/2), \quad (6.23)$$

$$\Psi^{II} (d/2) = \Psi^{III}_{k_x^+} (d/2).$$
6.3. A MAGNETIC FIELD STEP, SINGLE AND DOUBLE BARRIERS

From these relations we can connect $\Psi^I(d/2)$ with $\Psi^I(-d/2)$ with a matrix.

Figure 6.5: As in Fig. 6.3 for a magnetic barrier of width $d = 3l_B$.

Setting the determinant of this matrix equal to zero gives the dispersion relation. The resulting expressions are rather involved and will not be given here. Numerical results for the dispersion relation are given in Fig. 6.5 (a) and are contrasted with the corresponding ones for a single-layer barrier in Fig. 6.5(b). As in Fig. 6.3, we notice here the same difference in level spacing and the bending of the levels near the free particle result where $k_y$ is replaced by $k_y \pm d/2$ (red dashed curves). Notice that in contrast to the magnetic step case, where the spectrum is limited only from the right, now it is limited from the left as well and the pertinent $k_y$ values fall, approximately, in the range $-3 \leq k_y l_B \leq 3$.

Transmission

In contrast to the magnetic step problem where the transmission is zero for any value of the momentum, in the case of a magnetic barrier of finite width the transmission can attain non-zero values. To evaluate the transmission through a single magnetic barrier we write the solution in the three domains, denoted earlier, as follows. Region I ($x < -d/2$):

$$\Psi^I_{\pm} = \Psi^R_{E,\pm} + r^\pm \Psi^L_{E,\pm} + r^- \Psi^L_{E,-\pm}.$$ (6.24)

Region II ($-d/2 \leq x \leq d/2$):

$$\Psi^{II} = c_1 \Phi^-(z) + c_2 \Phi^-(-z) + c_3 \Phi^+(z) + c_4 \Phi^+(-z),$$ (6.25)

Region III ($x > d/2$):

$$\Psi^{III}_{\pm} = t^\pm \Psi^R_{E,\pm} + t^- \Psi^R_{E,-\pm}.$$ (6.26)
Figure 6.6: (a) Contour plot of the transmission $T$ through a magnetic barrier with $d = 2l_B$. The corresponding result for a single-layer graphene barrier is shown in (b). The angle $\theta$ is measured from the direction of normal incidence.

Here $r^\pm$ and $t^\pm$ are the reflection and transmission coefficients, respectively. After matching the solutions at $x = \pm d/2$ we obtain the transmission matrix as

$$t(E, q) = \begin{pmatrix} t_+^+(E, k_y) & t_+^-(E, k_y) \\ t_-^+(E, k_y) & t_-^-(E, k_y) \end{pmatrix},$$

and the transmission probability from

$$T = Tr(tt^\dagger).$$

A contour plot of the transmission probability is shown in panel (a) of Fig. 6.6 and is contrasted with that for a single-layer graphene barrier in panel (b). Comparing the two panels we see that in the bilayer case the angular range of perfect transmission becomes wider whereas the energy gap becomes narrower. For real wave vectors $k_x$, we can express the angular confinement of the transmission through a bilayer barrier as

$$-1 \leq \sin \theta^\pm \leq 1 - d/\sqrt{E^2 \pm Et},$$

where $\theta^\pm = \arctan [(k_y - d/2)/k^\pm]$. In Fig. 6.6(a) we have $\theta = \theta^+$ for $E > 0$ and $\theta = \theta^-$ for $E < 0$. The corresponding result for a single-layer barrier is obtained from Eq. (6.29) for $t^t = 0$. If we don’t use the dimensionless units, the last term in Eq. (6.29) is multiplied by $\lambda = h v_F / l_B$, i.e.,

$$d/E \rightarrow \lambda d/E, \ d/(E^2 \pm Et)^{1/2} \rightarrow \lambda d/(E^2 \pm Et)^{1/2}.$$
6.3. A MAGNETIC FIELD STEP, SINGLE AND DOUBLE BARRIERS

For a double barrier we proceed in the same manner as for a single one with the vector potential shown in the inset of Fig. 6.7 and given by

\[
A = \begin{cases} 
0, & x < -L/2 - d \\
(x + (L/2 + d))/d, & -L/2 - d \leq x \leq -L/2 \\
1, & -L/2 < x < L/2 \\
(x - (L/2 - d))/d, & L/2 \leq x \leq L/2 + d \\
2, & x > L/2 + d
\end{cases}
\]  

(6.31)

We obtain the transmission probability after matching the solutions at the four interfaces. In Fig. 6.7(a) we show a contour plot of the transmission, as a function of the angle of incidence and energy, and contrast it with that for the case of graphene in Fig. 6.7(b). We see again the same similarities and differences between the two panels that we saw in Fig. 6.6. In addition, upon comparing panels (a) in both figures we see how the gap widens and the angular range of perfect transmission shrinks upon increasing the number of barriers. Thus the allowed range of carriers that are able to transmit through both barriers is smaller than for a single magnetic barrier. Notice also that relative to the single-layer graphene, see Fig. 6.7(b), we

![Figure 6.7](image_url)

Figure 6.7: (a) Contour plot of the transmission \(T\) through a double magnetic barrier with \(d = l_B\) and \(L = 2l_B\). The result for single-layer graphene is shown in (b).

are forced, due to the linear spectrum, to consider wider intervals in energy to see any transmission.
6.3.3 Structures with \( <B> = 0 \)

Here we consider magnetic structures with inhomogeneous magnetic field profiles but such that the average magnetic field vanishes, i.e., with \( <B> = 0 \), and compare the transmission probability through them with that through the same single-layer structures with linear spectrum. Such magnetic field profiles are typically obtained when we overlay nanostructured ferromagnetic stripes on a graphene bilayer, see Fig. 2.15(a). In Fig. 6.8(a) we show a contour plot of the transmission probability for the structure shown in its inset for \( d = 3l_B \) and in Fig. 6.8(b) the corresponding single-layer result. In this case the transmission probability is symmetric with respect to the angle of incidence and the angular range for \( \theta \) is given by

\[
-1 + \frac{d}{\sqrt{E^2 \pm El'}} \leq \sin \theta \leq 1 - \frac{d}{\sqrt{E^2 \pm El'}}.
\]  

(6.32)

Beyond this range, there is still a nonzero tunneling because of the evanescent wave solutions inside the magnetic barrier. The result for single-layer graphene is obtained by setting \( l' = 0 \) in Eq. (6.32) and reads

\[
-1 + \frac{d}{E} \leq \sin \theta \leq 1 - \frac{d}{E}.
\]  

(6.33)

Again, Eq. (6.30) applies if we use the standard units.

In Fig. 6.9 we show a contour plot of the transmission for a two-unit structure, the unit shown in the inset of Fig. 6.8(a). Again panel (a) shows the bilayer result and panel (b) the single-layer one.
6.3. A MAGNETIC FIELD STEP, SINGLE AND DOUBLE BARRIERS

Notice that as compared to the simple double magnetic barrier structure (see Fig. 6.7) the transmission: 1) is even with respect to the angle of incidence, 2) exhibits a very rich set of resonances, and 3) is mainly nonzero for angles close to perpendicular incidence. The conductance of this double unit is shown in Fig. 6.10(b) and is contrasted with the one for a single unit (see Fig. 6.8(a)). Clear resonances are observed as a function of the Fermi energy of the particles. We compare these results with the corresponding one for the simple double magnetic barrier (see inset of Fig. 6.7(a)) in Fig. 6.10(a)) for two different inter-barrier distances. Only a very weak resonant structure is found when the magnetic barriers are separated over a larger distances. Notice also the zero conductance region for small Fermi energy which is absent in Fig. 6.10(b)) and which can be easily understood from the transmission plots (see Fig. 6.7).

\begin{figure}[h]
\centering
\includegraphics{figure6_9.png}
\caption{(a) Contour plot of the transmission $T$ through a unit twice that shown in Fig. 6.8(a) with $d = l_B$ and $L = 3l_B$. (b) As in (a) for the same structure on single-layer graphene.}
\end{figure}

6.3.4 Delta-function magnetic barriers

It is instructive to consider the limit of delta function magnetic barriers which considerably simplifies the calculations. For a single magnetic $\delta$-function barrier we have $B(x) = B_0 l_B \delta(x)$; the corresponding vector potential is $A(x) = B_0 l_B [\theta(x) - \theta(-x)]/2$, where $\theta(x)$ is the step function. Here we have two regions $x < 0$ and $x > 0$. The solution for regions I and II are

$$
\Psi_{I,\pm}^{\parallel} = \Psi_{E,\pm}^{\parallel} + r_+^{\pm} \Psi_{E,\pm}^{\parallel}, \quad (6.34)
$$

$$
\Psi_{II,\pm}^{\parallel} = t_+^{\pm} \Psi_{E,\pm}^{\parallel}. \quad (6.35)
$$
Figure 6.10: Conductance $G$ as a function of energy through a double magnetic barrier (inset of Fig. 6.7) with $d = l_B$ for two different $L$. (b) $G$ through the structure shown in Fig. 6.9(a) with $< B > = 0$, $d = l_B$ and $L = 10 l_B$. The inset shows $G$ through the structure shown in Fig. 6.8(a) with $d = 3 l_B$.

After matching the wavefunctions at $x = 0$, the transmission amplitudes $t^\pm_\pm$ can be combined in the transmission matrix given by Eq. (6.27); the transmission probability is given by Eq. (6.28).

For two magnetic $\delta$-function barriers (shown in Fig. 6.11(a)) the corresponding vector potential is

$$A(x) = B_0 l_B \begin{cases} 
0, & x < -L/2 \\
1, & -L/2 < x < L/2 \\
0, & x > L/2
\end{cases} \tag{6.36}$$

We consider three regions $I(x < -L/2)$, $II(-L/2 < x < L/2)$, and $III(x > L/2)$. The three solutions are

$$\Psi^I_\pm = \Psi^R_{E,\pm} + r^\pm_+ \Psi^L_{E,\pm} + r^\pm_- \Psi^L_{E,-}, \tag{6.37}$$

$$\Psi^{II}_\pm = c_1 \Psi^R_{E,\pm} + c_2 \Psi^R_{E,-} + c_3 \Psi^L_{E,\pm} + c_4 \Psi^L_{E,-}, \tag{6.38}$$

and,

$$\Psi^{III}_\pm = t^\pm_+ \Psi^R_{E,\pm} + t^\pm_- \Psi^R_{E,-}. \tag{6.39}$$

Here $k^I_x = [E^2 - (k_y + 1)^2]^{1/2}$, $k^II_x = k^I_x$, $k^III_x = k^I_x$. After matching at $x = -L/2$ and $x = L/2$ we can find the transmission matrix elements. Numerical results
6.4. CONCLUSIONS

We evaluated the transmission through various magnetic barrier nanostructures on bilayer graphene and contrasted it with that in the same structures on single-layer graphene. In particular, we treated a magnetic step, single and double regular or δ-function barriers as well as complex structures with inhomogeneous magnetic field profiles but such that the average magnetic field vanishes. To demonstrate the main new physics we limited ourselves to simple model magnetic field profiles that qualitatively approximate experimentally realizable nonhomogenous magnetic field profiles.

We showed that the transmission exhibits a strong dependence on the direction of the incident electron or hole wave vector. In general, the angular range of perfect...
transmission becomes drastically wider and the gaps drastically narrower. This perfect transmission range decreases with increasing number of barriers. Moreover, the transmission through the complex structures shows much more pronounced resonances than that through single or double barriers. To our knowledge these results are new.

An important feature of the transmission results is their dependence on the angle of incidence as shown in several figures and highlighted in Ref. [58] for a single barrier: the transmission is finite only in a certain range of angles of incidence, cf. Eqs. (6.29), (6.32), and (6.33). Given the connection between the wavevectors and $\theta$, this is equivalent to wavevector filtering or confinement. One can further modify the angular dependence of the transmission with double barriers, cf. Fig. 6.7. The main parameters that control this angular dependence are the width of the barriers/wells, the energy of the incident electrons, and the magnetic field, cf. Eq. (6.30). Given the rapid progress in the field and the quest for carbon-based nanostructure devices, we expect that the predictions/findings of this paper will be tested experimentally in the near future. We defer to future work the influence of spin and spin-orbit interaction in transport through these or similar graphene nanostructures.
Magnetic Kronig-Penney model for Dirac electrons in single-layer graphene

Abstract. The properties of Dirac electrons in a magnetic superlattice (SL) on graphene consisting of very high and thin ($\delta$-function) barriers are investigated. We obtain the energy spectrum analytically and study the transmission through a finite number of barriers. The results are contrasted with those for electrons described by the Schrödinger equation. In addition, a collimation of an incident beam of electrons is obtained along the direction perpendicular to that of the SL. We also highlight the analogy with optical media in which the refractive index varies in space.

7.1 Introduction

Given the importance of graphene, it would be appropriate to study this magnetic confinement more systematically. We make such a study here by considering a magnetic Kronig-Penney (KP) model in graphene, i.e., a series of magnetic $\delta$-function barriers that alternate in sign. This model can be realized experimentally in two different ways:

1) One can deposit ferromagnetic strips on top of a graphene layer but in a way that there is no electrical contact between graphene and these strips. When one magnetizes the strips along the $x$ direction, cf. Fig. 7.1(a), by, e.g., applying an in-plane magnetic field, the charge carriers in the graphene layer feel an inhomogeneous magnetic field profile. This profile can be well approximated [33] by $2B_0 z_0 h/(x^2 + z_0^2)$ on one edge of the strip and by $-2B_0 z_0 h/(x^2 + z_0^2)$ on the other, where $z_0$ is the distance between the 2DEG and the strip, and $d$ and $h$ the width and height of the strip (see Fig. 7.1(b)). The resulting magnetic field profile

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will be modeled by two magnetic $\delta$ functions of height $2\pi B_0 h$. Such ferromagnetic strips were deposited on top of a two-dimensional electron gas (2DEG) in a semiconductor heterostructure in Ref. [66].

2) It was recently shown that local strain in graphene induces an effective inhomogeneous magnetic field [67–69, 108] (Fig. 7.1(c)). When one puts the graphene layer on a periodically structured substrate the graphene at the edges of the substrate becomes strained and the situation can be described by a magnetic $\delta$-function profile such as that shown in Fig. 7.2.

In a quantum mechanical treatment of the above two systems the vector potential $A(x)$ is the essential quantity and, within the Landau gauge, $A(x)$ is nothing else than a periodic array of step functions. The Hamiltonian describing this system is periodic and consequently we expect the energy spectrum of the charge carriers in graphene to exhibit a band structure. The advantage of this magnetic Kronig-Penney (KP) model is mainly its analytical simplicity that provides some insight and allows a contrast with the same model for standard electrons [107]. To do that we adapt a method developed in optics, for a media with periodic in space refractive index. This optical method is clear and very well suited to the problem. Incidentally, there are many analogues of optical behavior in electronics, such as focusing [76–78, 96, 109], collimation or quasi-1D motion of electrons and photons [54, 58, 110, 111], and interference [84] in a 2DEG.

Figure 7.1: (a) Layout of the system: a ferromagnetic stripe on top of a bilayer graphene sheet separated by a thin oxide layer. (b) Magnetic field and corresponding vector potential at a distance $z_0 = 0.1$ under the stripe for parallel to it. (c) The graphene layer on top of a periodic structured surface.
7.2 Characteristic matrix for Dirac electrons

An electron in a single-layer graphene, in the presence of a perpendicular magnetic field \( B(x) \), which depends on \( x \), is adequately described by the Hamiltonian

\[
H_0 = v_F \sigma \cdot (p + eA(x)),
\]

(7.1)

where \( p \) is the momentum operator, \( v_F \) the Fermi velocity, and \( A(x) \) the vector potential. To simplify the notation we introduce the dimensionless units:

\[
\ell_B = \left[ \frac{\hbar}{eB_0} \right]^{1/2}, \quad B(x) \rightarrow B_0 B(x), \quad A(x) \rightarrow B_0 \ell_B A(x), \quad t \rightarrow t \ell_B / v_F, \quad r \rightarrow \ell_B r, \quad v \rightarrow v_F v, \quad E \rightarrow E_0 E, \quad u(x) \rightarrow E_0 u(x), \quad E_0 = \hbar v_F / \ell_B.
\]

Here \( \ell_B \) is the magnetic length and \( t \) the tunneling strength. In these units Eq. (7.1) takes the form

\[
H = \begin{pmatrix} 0 & \partial_x - i \partial_y + A(x) \\ \partial_x + i \partial_y - A(x) & 0 \end{pmatrix}.
\]

(7.2)

Then the equation \( H \Psi(x,y) = E \Psi(x,y) \) admits solutions of the form

\[
\Psi(x,y) = \begin{pmatrix} \psi_I(x,y) \\ \psi_{II}(x,y) \end{pmatrix},
\]

(7.3)

with \( \psi_I(x,y), \psi_{II}(x,y) \) obeying the coupled equations

\[
i \left[ \frac{\partial}{\partial x} - i \frac{\partial}{\partial y} + A(x) \right] \psi_{II} + E \psi_I = 0,
\]

(7.4)

\[
i \left[ \frac{\partial}{\partial x} + i \frac{\partial}{\partial y} - A(x) \right] \psi_I + E \psi_{II} = 0.
\]

(7.5)

Due to the translational invariance along the \( y \) direction we assume solutions of the form \( \Psi(x,y) = \exp ik_y y(U(x),V(x))^T \), with the superscript \( T \) denoting the transpose of the row vector. For \( B(x) \sim \delta(x) \) the corresponding vector potential is a step function \( A(x) \sim \Theta(x) \). For \( A(x) = P \) constant, Eqs. (7.4) and (7.5) take the form

\[
\frac{d}{dx} + (k_y + P) \quad V = iEU,
\]

(7.6)

\[
\frac{d}{dx} - (k_y + P) \quad U = iEV.
\]

(7.7)

Equations (7.3)-(7.7) correspond to those for an electromagnetic wave propagating through a medium in which the refractive index varies periodically. The two components of \( \Psi(x,y) \) correspond to those of the electric (or magnetic) field of
the wave [112, 113]. Equations (7.6) and Eq. (7.7) can be readily decoupled by substitution. The result is

\[ \frac{d^2Z}{dx^2} + \left[ E^2 - (k_y + P)^2 \right] Z = 0, \]  

(7.8)

where \( Z = U, V \). If \( E^2 \rightarrow E' \) and \((k_y + P)^2 \rightarrow V_{eff}\), Eq. (7.8) reduces to a Schrödinger equation for a standard electron where \( V_{eff}(k_y, x) = (k_y + P)^2 \) can be considered as an effective potential. Taking \( \theta_0 \) as the angle of incidence, we have

\[ k_x = E \cos \theta_0 = \left[ E^2 - k_y^2 \right]^{1/2} \]  

and

\[ k_y = E \sin \theta_0 \]  

are the wave vector components outside the medium and \( k'_x = E \cos \theta = \left[ E^2 - (k_y + P)^2 \right]^{1/2} \) is the electron wave vector inside the medium and \( \theta = \tan^{-1}(k_y/k'_x) \) is the refraction angle. This renders Eq. (7.8) simpler with acceptable solutions for \( U \) and \( V \):

\[ U(x) = A \cos \left( Ex \cos \theta \right) + B \sin \left( Ex \cos \theta \right), \]  

(7.9)

\[ V(x) = -i \left\{ B \cos \left( \theta + Ex \cos \theta \right) - A \sin \left( \theta + Ex \cos \theta \right) \right\}. \]  

(7.10)

For future purposes, we write \( U \) and \( V \) as a linear combination of \( U_1, U_2 \) and \( V_1, V_2 \):

\[ \frac{dV_1}{dx} + (k_y + P)V_1 = iEU_1, \quad \frac{dV_2}{dx} + (k_y + P)V_2 = iEU_2, \]  

\[ \frac{dU_1}{dx} - (k_y + P)U_1 = iEV_1, \quad \frac{dU_2}{dx} - (k_y + P)U_2 = iEV_2. \]  

(7.11)

We now multiply the equations of the first row by \( U_2 \) and \( U_1 \), respectively, and those of the second by \( V_2 \) and \( V_1 \). The resulting equations lead to

\[ \frac{dD}{dx} = U'_1V_2 + U_1V'_2 - V'_1U_2 - V_1U'_2 = 0, \]  

(7.12)

where \( D = detD \) and

\[ D = \begin{pmatrix} U_1 & V_1 \\ U_2 & V_2 \end{pmatrix}. \]  

(7.13)

Equation (7.12) shows that the determinant of the matrix (7.13) associated with any two arbitrary solutions of Eq. (7.8) is a constant, i.e, \( D \) is an invariant of the system of Eqs. (7.11). This also follows from the well-known property of the Wronskian of second-order differential equations. For our purposes the most convenient choice of particular solutions is

\[ U_1 = f(x), \quad U_2 = F(x), \]  

\[ V_1 = g(x), \quad V_2 = G(x), \]  

(7.14)
such that

\[ f(0) = g(0) = 0, \quad F(0) = G(0) = 1. \quad (7.15) \]

Then the solution with \( U(0) = U_0, \ V(0) = V_0 \), can be expressed as

\[ U = FU_0 + fV_0, \quad V = GU_0 + gV_0 \quad (7.16) \]

or, in matrix notation, as

\[ Q = \begin{bmatrix} U(x) \\ V(x) \end{bmatrix}, \quad Q_0 = \begin{bmatrix} U_0 \\ V_0 \end{bmatrix}, \quad N = \begin{bmatrix} F(x) & f(x) \\ G(x) & g(x) \end{bmatrix}. \quad (7.17) \]

Since \( D \) is constant, the determinant of the square matrix \( N \) is a constant; its value,

\[ \text{det} N = Fg - fG = 1. \]

It is usually more convenient to express \( U_0 \) and \( V_0 \) as a function of \( U(x) \) and \( V(x) \). Solving for \( U_0 \) and \( V_0 \) we obtain \( Q_0 = MQ \), where

\[ M = \begin{bmatrix} g(x) & -f(x) \\ -G(x) & F(x) \end{bmatrix}. \quad (7.18) \]

This matrix \( M \) is unimodular, \( |M| = 1 \). Now we can find the characteristic matrix from Eqs. (7.9) and (7.10) as

\[ M(x) = \frac{1}{\cos \theta} \begin{bmatrix} \cos (\theta + Ex \cos \theta) & -i \sin (Ex \cos \theta) \\ -i \sin (Ex \cos \theta) & \cos (\theta - Ex \cos \theta) \end{bmatrix}. \quad (7.19) \]
7.2.1 Bound states

Regards to the average of vector potential we shall consider two different systems: one with zero average and the other with non-zero average along the \( x \)-direction. First let us consider the magnetic field profile as shown in Fig. 7.2(a) for which the corresponding vector potential is

\[
A(x) = P\Theta(x)\Theta(L-x),
\]

(7.20)

where \( \Theta(x) = 0(x<0), 1(x>0) \) is the theta function. This vector potential has a non-zero average, and the corresponding effective potential becomes (see Fig. 7.3(a)) as

\[
V_{\text{eff}}(k_y, x) \sim \begin{cases} 
  k_y^2 & x < 0 \\
  (k_y + P)^2 & 0 < x < L \\
  k_y^2 & x > L
\end{cases}
\]

(7.21)

Here \( L \) is measured in the unit of magnetic length \( l_B \). There are two different cases which we have to consider.

Case 1 for \( k_y < -P/2 \): as shown in Fig. 7.3(a) by the full red curve, we have a 1D symmetric quantum well which, as is well-known, has at least one bound state.
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(see also Fig. 7.3(c)). For \( E^2 < k_y^2 \) the particle will be bound while for \( E^2 > k_y^2 \) we have scattered states, or equivalently the electron tunnels through the magnetic barriers.

Case 2 for \( k_y > -P/2 \): as shown in Fig. 7.3(a) by the dotted blue curve, the effective potential is like a barrier. We have a pure tunneling problem. With reference to Fig. 7.2, \( x_1 = 0 \) and \( x_2 = L \), the solutions are as follows. For \( x < 0 \) the wave function is

\[
\psi(x) = Ce^{\kappa x} \left( \frac{1}{1-e^{-\xi}} \right),
\]

where \( \kappa = E \cosh \xi \) and \( k_y = E \sinh \xi \), while for \( x > L \) it is

\[
\psi(x) = De^{-\kappa x} \left( \frac{1}{ie^\xi} \right).
\]

In the middle region, \( 0 < x < L \), the wave function is given by

\[
\psi(x) = Fe^{ik'y} \left( \frac{1}{e^{i\theta}} \right) + Qe^{-ik'y} \left( \frac{1}{1-e^{-i\theta}} \right).
\]

With \( k' = \left[ E^2 - (k_y + P)^2 \right]^{1/2} = E \cos \theta \). Matching the wave functions at \( x = 0 \) and \( x = L \) leads to a system of four equations relating the coefficients \( C, D, F, \) and \( Q \). Setting the determinant of these coefficients equal to zero, we obtain the transcendental equation, the solution of it gives the energy spectrum

\[
\cos \theta \cosh \xi \cos k'L + \sin \theta \sinh \xi \sin k'L = 0.
\]

For the special value of \( k_y = -P \), \( \sin \theta = 0 \), and we can rewrite Eq. (7.25) as \( \cos (EL) = 0 \) or equally \( E_n = \left( n + \frac{1}{2} \right) \frac{\pi}{L} \). The resulting bound states, as a function of \( k_y \), are shown by the red full curves in Fig. 7.4(a). The area of existence of bound states is delimited by the lines \( E = -k_y \) and \( E = -(k_y + P) \). The number of bound states increases with \( |k_y| \) which is also clear from the behavior of the min. and max. of the effective potential (see Fig. 7.3(c)). No bound states are found for \( k_y > -P/2 \) as is also apparent from Fig. 7.3(c). For \( k_y \to -P/2 \) the potential is shallow and only one bound state exists. The average velocity \( v_n(k_y) \) along the \( y \) direction is given by

\[
v_n(k_y) = \partial E / \partial k_y = \int_{-\infty}^{+\infty} dx j_y(x),
\]

where \( j_y = -i(U^*V - V^*U) \). From Fig. 7.4(a) it is clear that these bound states move along the \( y \)-direction, i.e. along the magnetic barriers. Their velocity \( v_y >
\(-v_F\) is negative for \(k_y < -P\) but as the electron is approaching \(k_y \rightarrow -P\) we have \(v_y \rightarrow 0\). For \(k_y > -P\) the velocity \(v_y > v_F\) is positive. This can be understood from the maximum and minimum of the effective potential which is shown in Fig. 7.3(c). The energy bound states can only exist between these two lines. Notice that the slope of \(V_{\text{eff}}\) is negative for \(k_y < -P\) while it turns positive for \(k_y > -P\) which explains the \(k_y\) dependence of the velocity. From Fig. 7.4(a) it is clear there are two different classes of bound states. The bound state which follows very closely the \(k_y = -P\) curve and extends to the region \(-P < k_y < 0\) with energy close to zero has a wavefunction that is concentrated around the position of the two magnetic delta function and decays exponentially in the region \(0 < x < L\). The wave function of the other bound states are concentrated in a region between the two magnetic delta-functions (i.e. like in a standing wave fashion) and decays exponentially outside this region.

Next, we consider a structure with zero-average vector potential as shown in Fig. 7.2(b), with corresponding effective potential shown in Fig. 7.3(b). The effective potential for \(k_y < -P/2\) and \(k_y > P/2\), consist of a potential well and a potential barrier and therefore has at least one bound state. Thus we expect bound states for all \(k_y\) with energy between \(E = -(+)(k_y + P)\) and \(E = -(+)k_y\) when \(k_y < -P/2\) \((k_y > P/2)\). The dispersion relation for those bound states are the solution of

\[
M_{21} - M_{12} - iM_{22}e^{-\xi} - iM_{11}e^{\xi} = 0, \quad (7.27)
\]

where \(M\) is the transfer matrix for the unit shown in Fig. 7.2(d). These bound states are shown by the red full curves in Fig. 7.4(b). Because of the spatial inversion
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Figure 7.5: (a) Transmission vs energy through the magnetic δ-function barriers of in Fig. 7.4(a) \( k_y = -0.05 \). (b) same as (a) but now for the configuration shown in Fig. 7.2(b) for \( k_y = 0 \). (c) Transmission vs \( k_y \) through the system described in Fig. 7.4(a) for fixed \( E = 0.1 \). The red arrow lines indicate the position of the bound states. (d) same as (c) but now for the configuration shown in Fig. 7.2(b) for \( E = 0.15 \).

symmetry of the vector potential the spectrum has the symmetry \( E(-k_y) = E(k_y) \). Notice that for \(-P < k_y < P\) the lowest bound state has energy \( E \approx 0 \). For \(-P/2 < k_y < P/2\) we have two potential barriers and therefore no bound states.

7.2.2 Reflection and transmission coefficients

Consider a plane wave incident upon a system of two δ-function magnetic barriers, identical in height but opposite in direction, placed at \( x = 0 \) and \( x = L \), as shown schematically in Fig. 7.2(a). In this case the vector potential is constant for \( 0 \leq x \leq L \), zero outside this region, and homogeneous in the \( y \) direction. Below we derive expressions for the amplitudes and intensities of the reflected and transmitted waves.

Let \( A, R, \) and \( T \) denote the amplitudes of the incident, reflected, and transmitted waves, respectively. Further, let \( \theta_0 \) be the angle of incidence and exit as shown
Figure 7.6: Contour plot of the transmission (a) and Bloch phase (c) through $N = 10$ magnetic $\delta$-function barriers with $a = 10$, $b = 10$, and $P = 1$. (b) and (d) The same as in (a) and (c) for $a = 5$, $b = 5$, $c = 5$, $d = 5$, and $P = 1$, single unit.

In Fig. 7.2(b). The boundary conditions give

$$
U_0 = A + R, \quad U(L) = T e^{i kl}, \quad V_0 = A e^{i \theta_0} - Re^{-i \theta_0}, \quad V(L) = e^{i \theta_0} e^{ikh} T. \quad (7.28)
$$

The four quantities $U_0, V_0, U,$ and $V$ given by Eqs. (7.28) are connected by the basic relation $Q_0 = MQ$; hence, with $J = m'_{11} + m'_{12} e^{i \theta_0}$ and $K = m'_{21} + m'_{22} e^{i \theta_0}$, we have

$$
A + R = JT e^{i kl}, \quad Ae^{i \theta_0} - Re^{-i \theta_0} = KTe^{i kl}, \quad (7.29)
$$

where $m'_{ij}$ are the elements of the characteristic matrix of the medium, evaluated at $x = L$. From Eq. (7.29) we obtain the reflection and transmission amplitudes

$$
r = \frac{R}{A} = \frac{Je^{i \theta_0} - K}{Je^{-i \theta_0} + K}, \quad t = \frac{T}{A} = \frac{2e^{-ikh \cos \theta_0}}{Je^{-i \theta_0} + K}. \quad (7.30)
$$

In terms of $r$ and $t$ the reflectivity and transmissivity are

$$
R = |r|^2, \quad T = |t|^2. \quad (7.31)
$$
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The characteristic matrix for a homogeneous vector potential is given by Eq. (7.19). Labeling with subscripts 1, 2, and 3 quantities which refer to the regions, respectively, I, II, and III of Fig. 7.2(a), and by \( L = x_2 - x_1 \) distance between the magnetic \( \delta \)-functions, we have

\[
\begin{align*}
m'_{11} &= \cos (\theta_i + \beta) / \cos \theta_i, \quad m'_{22} = \cos (\theta_i - \beta) / \cos \theta_i, \\
m'_{12} &= -i \sin \beta / \cos \theta_i, \quad m'_{21} = -i \sin \beta / \cos \theta_i.
\end{align*}
\]

The reflection and transmission amplitudes \( r \) and \( t \) are obtained by substituting these expressions in those for \( J \) and \( K \) that appear in Eq. (7.30). The resulting formula can be expressed in terms of the amplitudes \( r_{12}, t_{12} \) and \( r_{23}, t_{23} \) associated with the reflection at and transmission through the first and second "interface", respectively. We have

\[
\begin{align*}
r_{12} &= e^{i\theta_0} - e^{i\theta_i} \frac{e^{-i\beta} + e^{i\beta}}{e^{-i\theta_0} + e^{i\theta_i}}, \\
t_{12} &= \frac{2 \cos \theta_0}{e^{-i\theta_0} + e^{i\theta_i}}, \quad t_{12} = 2 \cos \theta_0 \\
\end{align*}
\]

and similar expressions for \( r_{23} \) and \( t_{23} \). In terms of these expressions \( r \) and \( t \) become

\[
\begin{align*}
r &= \frac{r_{12} + r_{23} e^{2i\beta}}{1 + r_{12} r_{23} e^{2i\beta}}, \\
t &= \frac{t_{12} t_{23} e^{2i\beta}}{1 + r_{12} r_{23} e^{2i\beta}}.
\end{align*}
\]

The amplitude \( t \) of the transmission through the system is given by [58,59,61,108],

\[
t = \frac{2 e^{-i k L \cos \theta_0 \cos \theta_i}}{e^{-i \beta} [\cos (\theta_0 + \beta) + 1] + e^{i \beta} [\cos (\theta_0 - \beta) - 1]},
\]

Figure 7.7: (a) and (b) Transmission vs energy through \( N = 1, 5, 10 \) magnetic units of \( \delta \)-function barriers shown on the left. The upper unit has \( a = 10, b = 10, P = 1, E = 1.5 \) and the bottom one \( a = b = c = d = 5, P = 1 \) and \( E = 2.5 \).
where $k_y = E \sin \theta_0$, and $k_y + P = E \sin \theta_i$. This equation remains invariant under the changes $E \rightarrow -E$, $\theta_0 \rightarrow -\theta_0$, $\theta_i \rightarrow -\theta_i$. A contour plot of the transmission is shown in Fig. 7.4(a) and slices for constant $k_y$ and $E$ are shown respectively in Fig. 7.5(a) and Fig. 7.5(b). By imposing the condition that the wave number $k_x$ be real for incident and transmitted waves, we find that the angles $\theta_0$ and $\theta_i$ are related by

$$\sin \theta_0 + \frac{P}{E} = \sin \theta_i.$$  

(7.36)

Equation (7.36) expresses the angular confinement of the transmission elaborated in Refs. [58, 59, 61, 114]. Notice its formal similarity with Snell’s law. Using Eq. (7.36) we obtain the range of incidence angles $\theta_0$ for which transmission through the first magnetic barrier is possible

$$-1 - \frac{P}{E} \leq \sin \theta_0 \leq 1 - \frac{P}{E}.$$  

(7.37)

For the special value of the energy $E = P/2$ and $\theta_0$ in the range $-\pi/2 \leq \theta_0 \leq \pi/2$, we have $\theta_i = \pi/2$ while for $E = -P/2$ the result is $\theta_i = -\pi/2$. Alternatively, we can put $\theta_i = \pm \pi/2$ in Eq. (7.36) and obtain, for $P > 0$, the result

$$\sin \theta_0^{\pm} = \pm 1 - \frac{P}{E},$$  

(7.38)
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Figure 7.9: Dispersion relation ($E$ vs $k$) for a standard electron in (a) and a Dirac electron in (b). The fixed values of $k_y$ are shown in the panels and $L = 8$ and $P = 1$ (the energy for standard electron is measured in units of $\hbar\omega_c$ with $\omega_c = \sqrt{eB_0/mc}$ and all distances in $l_B = \sqrt{\hbar/eB_0}$).

where the $+(-)$ sign corresponds to $E > 0$ ($E < 0$). A contour plot of the transmission as function of $E$ and $k_y$, obtained from Eq. (7.35), is shown in Fig. 7.4(a). In Fig. 7.4(a) we distinguish three different regions. In the region between $E = -(k_y + P/2)$ and $E = -k_y$, the wave vector of the incident wave is imaginary and they are evanescent waves. In this region $k'$ is real and it is possible to find localized states. The $k$ and $k'$ for the second region between $E = k_y + P/2$ and $E = -(k_y - P/2)$ are real and the electron can tunnel through the magnetic $\delta$-barriers. In the blue shadow region between $E = k_y + P/2$ and $E = k_y - P/2$, $k$ is real but $k'$ is imaginary and solutions inside the barrier are evanescent and there is very little tunneling which becomes very quickly zero. The transmission probability $|T| = t \cdot t^*$ is equal to 1 for $\cos (2\beta) = 1$. In this case the energy becomes

$$E_n = \pm \left[ n^2\pi^2/L^2 + (k_y + P)^2 \right]^{1/2}, \quad n = 1, 2, \ldots \quad (7.39)$$

The condition $\cos (2\beta) = 1$, or equivalently $\beta = n\pi = E\hbar\cos \theta_2$ with $n$ an integer, should be combined with that for the transmission to occur in the region delimited by the curves $E = \pm(k_y + P)$ and $E = \pm k_y$. For example, in Fig. 7.4(a) for $k_y = -0.05$ and $0 < E < 0.2$ we have 12 maxima. It is readily seen that with these parameters in Eq. (7.39) we find 12 different energies as shown in Fig. 7.5(a). Fig. 7.4(b) shows a contour plot of the transmission for the structure shown in Fig. 7.4(b).
7.2(d), which is symmetric around $k_y = 0$. Notice that the number of resonances has increased substantially as compared to previous case which is due to the fact that we have twice as many magnetic barriers in our systems.

### 7.3 A series of units with magnetic $\delta$-function barriers

#### 7.3.1 $N$ units

We consider a system of $N$ units, such as those shown in Fig. 7.2(a) and Fig. 7.2(d) with periods $L = a + b$ and $L = a + b + c + d$, respectively. The corresponding periodic vector potential is $A(x) = A(x + nL)$ and the magnetic field $B = B(x + nL)$, with $n = 1, 2, ..., N$. The characteristic matrix for one period $M(L)$ is denoted by

$$M(L) = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix}. \quad (7.40)$$

On account of the periodicity we have

$$M(NL) = M(L) \cdot M(L) \cdot ... \cdot M(L) = (M(L))^N. \quad (7.41)$$

To evaluate the elements of $M(NL)$ we use a result from the theory of matrices, according to which the $N$th power of a unimodular matrix $M(L)$ is $(u_N(\chi) \equiv u_N)$

$$[M(L)]^N = \begin{bmatrix} m_{11}u_{N-1} - u_{N-2} & m_{12}u_{N-1} \\ m_{21}u_{N-1} & m_{22}u_{N-1} - u_{N-2} \end{bmatrix}, \quad (7.42)$$

with $\chi = \frac{1}{2}TrM$ and $u_N$ the Chebyshev polynomials of the second kind:

$$u_N(\chi) = \sin[(N + 1)\zeta]/\sin \zeta, \quad (7.43)$$

where

$$\zeta = \cos^{-1} \chi, \quad (7.44)$$

Here $\zeta$ is the Bloch phase of the periodic system [115], which is related to the eigenfunctions of $M$. In the limit case of $N \to \infty$, we have total reflection when $\zeta$ is outside the range $(-1, 1)$. 

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Figure 7.10: First energy band for (a) standard and (c) Dirac electron in SL of magnetic $\delta$-function barriers with $a = 100$, $b = 100$, and $P = 0.1$. (b) and (d) corresponding contour plots of (a) and (c) (the energy for standard electron is measured in units of $\hbar\omega_c$ with $\omega_c = \sqrt{eB_0/mc}$ and all distances in $l_B = \sqrt{e\hbar/cB_0}$).

7.3.2 Superlattice

Here we consider a finite number $N$ of lattice unit shown in Fig. 7.2(c). We set

$$\beta_2 = Eb \cos \theta_2, \quad \beta_1 = Ea \cos \theta_1, \quad p_2 = 1/\cos \theta_2,$$
$$p_1 = 1/\cos \theta_1, \quad h = a + b, \quad \lambda_n^\pm = \theta_n \pm \beta_n. \quad (7.45)$$

The characteristic matrix $M_2(L)$ for one period is readily obtained, in terms of these quantities, as in Sec. II, and from that the characteristic matrix $M_{2N}(NL)$ of the multilayer system according to Eq. (7.41). Its elements are

$$M_{11} = s[\cos \lambda_n^+ \cos \lambda_n^- - \sin \beta_2 \sin \beta_1]u_{N-1} - u_{N-2},$$
$$M_{12} = -isu_2[\sin \lambda_n^+ \sin \beta_1 + \sin \beta_2 \cos \lambda_n^-]u_{N-1},$$
$$M_{21} = -isu_2[\cos \lambda_n^- \sin \beta_2 + \sin \beta_1 \cos \lambda_n^+]u_{N-1},$$
$$M_{22} = s[\cos \lambda_n^- \cos \lambda_n^- - \sin \beta_2 \sin \beta_1]u_{N-1} - u_{N-2}, \quad (7.46)$$

where $s = p_2p_1$, $u_N \equiv u_N(\chi)$, and

$$\chi = \cos (k_1a) \cos (k_2b) - \left(\frac{k_2^2 + k_1^2 + P^2}{2k_2k_1}\right) \sin (k_1a) \sin (k_2b). \quad (7.47)$$
The reflection and transmission coefficients of the multi-unit system are immediately obtained by substituting these expressions into Eq. (7.30). The numerical results are shown in Figs. 7.6, 7.7 for finite superlattice with $N = 10$ units. Two different type of structures are considered as shown in the insets to Figs. 7.7. The transmission doesn’t have $k_y \to -k_y$ symmetry for the periodic system with magnetic delta up-down as is apparent from Fig. 7.7(a). We contrast these results with the case in which we used an arrangement of magnetic delta-function as in previous structure plus another unit with opposite direction of magnetic delta function. As is clearly shown in Fig. 7.7(b), we have $k_y \to -k_y$ symmetry for the transmission probability through this structure. The transmission resonances are more pronounced, i.e., the dips become deeper, when the number of barriers increases for both types of units. But the gaps occur when the wave is mostly reflected. The position of these gaps, which are especially pronounced as N increases, can also be found from the structure of the Bloch phase $\zeta$, as shown in Figs. 7.6(c) and (d). In Fig. 7.6 the bound states are shown by the blue solid curves that are situated in the area $-k_y - P/2 < E < -k_y + P/2$ in case (a) and in $-k_y - P/2 < E < -k_y$ for case (b) plus an area located symmetric with respect to $k_y$. Notice in Fig. 7.6(a) that several bound states merge into a resonant states at $E = -k_y + P/2$. This is different from Fig. 7.4(a) where each bound state becomes a resonant state at $E = -k_y$. 

Figure 7.11: Dispersion relation for a (a) standard electron and a (b) Dirac electron. The period is $L = a + b = 8$ and the shaded (in green) regions are the lowest six allowed bands. The solid curves in both panels, the dash-dotted curves in (a) and the dashed ones in (b) show bound states for free electron (the energy for standard electron is measured in units of $\hbar \omega_c$ with $\omega_c = \sqrt{eB_0/mc}$ and all distances in $l_B = \sqrt{\hbar/eB_0}$).
7.3. A SERIES OF UNITS WITH MAGNETIC $\delta$-FUNCTION BARRIERS

![Figure 7.12: Energy vs period $L = a + b$ for (a) standard electron and (b) Dirac electron with fixed $k_y = 4$ (the energy for standard electron is measured in units of $\hbar\omega_c$ with $\omega_c = \sqrt{eB_0/mc}$ and all distances in $l_B = \sqrt{\hbar/eB_0}$).](image)

7.3.3 Spectrum of a superlattice

Let's take $N \to \infty$. We can find the energy-momentum relation from the previous standard calculation [115, 116] by using

$$\cos(k_xL) = \frac{1}{2} TrM = \chi,$$

(7.48)

where $M$ is the characteristic matrix of one period, which results into

$$\cos (k_1a) \cos (k_2b) - \left(\frac{k_2^2 + k_1^2 + P^2}{2k_2k_1}\right) \sin (k_1a) \sin (k_2b) = \cos k(b + a).$$

(7.49)

With reference to the regions I and II shown in Fig. 7.2(a), we write $k_1 = [E^2 - k_y^2]^{1/2}$ and $k_2 = [E^2 - (k_y + P)^2]^{1/2}$ and show the solution for $E^2 > (k_y + P)^2$ in Fig. 7.10. Differences of Eq. (7.49) from the corresponding result of Ref. [107], Eq. (7.7), for the case of Schrödinger electrons, is the term $P^2$ in the prefactor of the second term on the right-hand side and the linear $E$ vs $k$ spectrum instead of the quadratic one in Ref. [107]. If $P$ is large the differences become more pronounced.

Our numerical results for the energy spectrum are shown in Figs. 7.8, 7.9, 7.10, 7.11, and 7.12. The results for standard and Dirac electrons show similarities but also important differences. The first band shows a qualitative difference near $k_y \approx 0$, see Fig. 7.10. As Figs. 7.8, 7.10(a) and 7.10(b) show, the band behavior in the $k = k_x$ direction for fixed $k_y$ is constant and almost symmetric about $k_y = 0$; the motion becomes nearly 1D for relatively large $k_y$. From the contour plots of Figs. 7.10(b) and (d), as well as from Fig. 7.8(c), we infer a collimation along the $k_y$ direction, i.e., $v_y \propto \partial E/\partial k_y \approx v_F$ and $v_x \approx 0$, which is similar to that found...
for a SL of electric potential barriers [111] for some specific values of the barrier heights. Also there are no gaps for \( k_y \approx 0 \) in Fig. 7.11(a) but there are for the case of Dirac electrons as seen in Fig. 7.11(b). This difference can be traced back to the presence of \( P^2 \) in the dispersion relation Eq. (7.49) when compare to the same equation for the standard electron. The even-number energy bands in Fig. 7.12(b) are wider than those in Fig. 7.12(a) and, as a function of the period, the energy decreases faster for Dirac electrons. This behavior of the bands for Dirac electrons is very similar to that for the frequency \( \omega \) vs \( k_y \) or \( L \) in media with a periodically varying refractive index [113]. This is clearly a consequence of the linear \( E - k \) relation. Notice the differences between the lowest bands shown in panels (a) and (b) in Fig. 7.13 and in particular the difference between the corresponding drift velocities as functions of \( k_y \).

### 7.4 Concluding remarks

We developed a magnetic Kronig-Penney model for Dirac electrons in graphene. The model is essentially a series of very high and very narrow magnetic \( \delta \)-function
barriers alternating in signs. The treatment of the transmission through such a series of barriers followed closely the one developed in optics for media in which the refractive index varies in space \[112, 113\]. We contrasted a few of the results with those for standard electrons described by the Schrödinger equation \[107\].

In several cases the energy spectrum or the dispersion relation were obtained analytically, largely due to the simplicity of the model and the adapted method from optics. For only two magnetic \(\delta\)-function barriers, opposite in sign, we saw several bound states, whose number increases with \(|k_y|\), and a reduction of the wavevector range for which tunneling is possible, cf. Fig. 7.4(a). This is in line with that reported earlier for single \[57\] and multiple \[59\] barriers. The reduction becomes stronger as we increase the number of barriers, cf. Fig. 7.4(b). We also made contact with Snell’s law in optics, cf. Eq. (7.36): the term \(P/E\) represents the deviation from this law.

An important feature of the superlattice results is a collimation of an incident electron beam normal to the superlattice direction at least for large wave vectors. As easily seen from Figs. 7.8 and 7.9, for \(|k_y| \geq 2\) we have \(v_x \propto \partial E/\partial k_x \approx 0\) for the first three minibands in the middle panels and nearly five minibands in the right panels. This occurs for both standard electrons and Dirac electrons but notice an important difference for \(|k_y| \approx 0\) shown clearly in Fig. 7.10. This collimation is similar to that reported in Ref. [111] for superlattices involving only electric barriers but with somewhat unrealistic large barrier heights.

It is also worth emphasizing the differences and similarities in the first two minibands and the corresponding drift velocities as functions of \(k_y\) for different periods \(L\) and constant \(k_x\) as shown in Fig. 7.13. Notice in particular the resemblance between the drift velocities in the lowest miniband for standard electrons and the second miniband for Dirac electrons.
8

Kronig-Penney model of scalar and vector potentials in graphene

Abstract. We consider a one-dimensional (1D) superlattice (SL) on graphene consisting of very high and very thin (δ-function) magnetic and potential barriers with zero average potential and zero magnetic field. We calculate the energy spectrum analytically, study it in different limiting cases, and determine the condition under which an electron beam incident on a SL is highly collimated along its direction. In the absence of the magnetic SL the collimation is very sensitive to the value of $W/W_s$ and is optimal for $W/W_s = 1$, where $W$ is the distance between the positive and negative barriers and $L = W + W_s$ the size of the unit cell. In the presence of only the magnetic SL the collimation decreases and the symmetry of the spectrum around $k_y$ is broken for $W/W_s \neq 1$. In addition, a gap opens which depends on the strength of the magnetic field. We also investigate the effect of spatially separated potential and magnetic δ-function barriers and predict a better collimation in specific cases.

8.1 Introduction

In this chapter, we consider a SL in which potential and magnetic barriers, with zero average potential and magnetic field, are present at the same time (see Fig. 8.1). We study the limit of δ-function barriers, that is, the Kronig-Penney (KP) limit, because it has the advantage that a lot can be done analytically and provides an insightful contrast with the same model for standard electrons [107]. In recent work it was shown that such a structure can create a gap in the band structure. This gap depends on the strength of the scalar and vector potentials [117]. Further, we investigate the effect of a magnetic SL on electron collimation and the properties

*The results of this chapter were published as:
of the energy gap. We studied also the case when the magnetic and potential SLs are shifted with respect to each other, see Fig. 8.1 for $a_s \neq 0$. All these aspects were not studied in our previous works, Refs. [81] and [82]: the former focused on periodic properties in a KP model of potential barriers and the latter on the energetics of a KP model of magnetic barriers. Here we consider the situation that both types of barriers are present at the same time which may displaced with respect to each other. We detail their physical consequences, mainly those on electron collimation and the energy gap created in such structures.

8.2 General formalism

The low-energy quasiparticles (electrons and holes) of a single-layer graphene in the presence of a perpendicular magnetic field $B(x)$ and external potential $V(x)$ are described by the Dirac-type Hamiltonian

$$H = v_F \sigma \cdot (p + eA(x)) + V(x);$$

(8.1)
8.2. GENERAL FORMALISM

Figure 8.2: profile of the perpendicular magnetic field component (solid curve) in the graphene layer and corresponding vector potential at a distance $z_0 = 0.1$ under the magnetic stripe for parallel magnetization.

Here $\sigma = (\sigma_x, \sigma_y)$ are the Pauli matrices, $\mathbf{p}$ the momentum operator, $v_F$ the Fermi velocity, and $A(x)$ the vector potential. The energy spectrum is obtained from the equation $H\Psi = E\Psi$ where

$$\Psi(x,y) = \begin{pmatrix} \psi_I(x,y) \\ \psi_{II}(x,y) \end{pmatrix}, \quad (8.2)$$

is the one-electron wave function. For periodic electric and vector potentials we denote the energy spectrum by $E_n(k_x, k_y)$ with $k = (k_x, k_y)$ the electron wave vector and $n$ the miniband index. To simplify the notation we introduce the dimensionless units: $B(x) \rightarrow B_0B(x)$, $A(x) \rightarrow B_0LA(x)$, $t \rightarrow t\ell/v_F$, $r \rightarrow \ell r$, $\mathbf{v} \rightarrow v_F\mathbf{v}$, $V \rightarrow E_0V$, $E \rightarrow E_0E$, $E_0 = \hbar v_F/\ell$, and set $\beta = eB_0\ell^2/\hbar$ with $\ell = 1\text{nm}$, $L = W + W_s$, $w = W/L$ and $w_s = W_s/L$.

Density of states (DOS). The number of k-states per unit energy is given by,

$$D(E) = \frac{1}{(2\pi)^2} \sum_n \int dk_xdk_y \delta(E - E_n(k_x, k_y)). \quad (8.3)$$

To calculate the DOS numerically we introduce a Gaussian broadening,

$$\delta(E - E_n(k_x, k_y)) \rightarrow \frac{1}{\Gamma\sqrt{\pi}} \exp \left[ -\frac{(E - E_n(k_x, k_y))^2}{\Gamma^2} \right]. \quad (8.4)$$

Conductivity. For elastic scattering the diffusive conductivity $\sigma_{ij}$ is given by

$$\sigma_{ij} = \frac{e^2}{4\pi^2 k_B T} \sum_n \int dk_xdk_y \tau v_{ni}v_{nj}f_{nk}(1 - f_{nk}) \quad (8.5)$$
Here $T$ is the temperature, $v_{ni} = \frac{\partial E_n}{\partial k_i}$ the electron velocity, $f_{nk}$ the Fermi-Dirac function, and $\tau$ the momentum relaxation time. For low temperatures we assume that $\tau$ is approximately constant, evaluated at the Fermi level ($\tau \approx \tau_F$), and replace the product $f_{nk}(1 - f_{nk})/k_B T$ by the delta function $\delta(E - E_n(k_x,k_y))$.

8.3 KP model: a SL of magnetic and potential $\delta$-function barriers

8.3.1 Formalism

Many properties of the electron bands resulting from a periodic potential can be investigated through the KP model which is exactly solvable. We consider a superlattice (SL) of magnetic and potential barriers as shown in Fig. 8.1. In this work we limit ourselves to potential and magnetic superlattices which have the same periodicity. First we consider the situation depicted in Fig. 8.1 where both SLs are in phase (i.e. $a_s = 0$). The vector potential profile for a single unit shown in Fig. 8.3(a) is

$$A(x) = (\beta/2)[\Theta(x)\Theta(W - x) - \Theta(-x)\Theta(x - W)] \quad (8.6)$$

The corresponding magnetic field is

$$B = \beta \ell[\delta(x) - \delta(x - W)]. \quad (8.7)$$

The potential profile is taken as

$$V(x) = P[\delta(x - W) - \delta(x)]. \quad (8.8)$$
where $P$ is the strength of the barrier. In region I of the single unit the wave function is given by

$$
\psi_I(x, y) = e^{ik_1 y} \begin{cases}
A e^{k_1 x}, & x < 0, \\
B e^{-k_1 x}, & x > W,
\end{cases}
$$

(8.9)

and in region II by

$$
\psi_{II}(x, y) = e^{ik_2 y} \begin{cases}
-iA e^{k_1 x - \theta}, & x < 0, \\
B e^{-k_1 x + \theta}, & x > W.
\end{cases}
$$

(8.10)

Here $\tanh \theta = (k_y - \beta/2)/k_1$, $\tan \varphi = (k_y + \beta/2)/k_2$, $k_1^2 = E^2 - (k_y - \beta/2)^2$, and $k_2^2 = E^2 - (k_y + \beta/2)^2$. The transfer matrix through a single $\delta$-function potential barrier is given by [81],

$$
M_d = \begin{bmatrix}
\cos P & i \sin P \\
-i \sin P & \cos P
\end{bmatrix},
$$

(8.11)

and that for barrier with the opposite sign is obtained by replacing $P$ with $-P$. The coefficients on the left and right hand side of the single unit are connected by

$$
A \left( \begin{array}{c}
1 \\
-ie^{-\theta}
\end{array} \right) = M_T \left( \begin{array}{c}
1 \\
-ie^\theta
\end{array} \right) Be^{-kW},
$$

(8.12)

where $M_T = M_d(-P)M_{W,\varphi}M_d(P)$ and $M_{W,\varphi}$ is the characteristic matrix inside the vector potential barrier given by [82],

$$
M_{W,\varphi} = \frac{1}{\cos \varphi} \begin{bmatrix}
\cos \lambda^+ & -i \sin \eta \\
-i \sin \eta & \cos \lambda^-
\end{bmatrix},
$$

(8.13)

with $\lambda^\pm = \varphi \pm EW \cos \varphi$ and $\eta = EW \cos \varphi$. The elements of $M_T$ can be readily obtained from those of $M_d(-P)$, $M_{W,\varphi}$, and $M_d(P)$. Then setting the determinant of the coefficients in Eq. (8.12) equal to zero leads to

$$
1 - \cos \varphi \cot \eta \sinh \theta - \sin \varphi \cosh \theta \cos(2P) = 0,
$$

(8.14)

which is similar to Eq. (25) in Ref. [82]. The solution of Eq. (8.14) gives the spectrum.

Next we consider a system of $N$ units, such as those shown in Fig. 8.1, with period $L = W + W_s$. The corresponding periodic scalar and vector potentials are
A(x) = A(x + nL) and V(x) = V(x + nL) and the magnetic field B = B(x + nL), with n an integer. The characteristic matrix for one period M(L) is denoted by

\[ M(L) = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix}. \]  

(8.15)

On account of the periodicity we have

\[ M(NL) = M(L) \cdot M(L) \cdot \ldots \cdot M(L) = (M(L))^N. \]  

(8.16)

To evaluate the elements of M(NL) we use a result from the theory of matrices, according to which the Nth power of a unimodular matrix M(L) is

\[ (M(L))^N = \begin{bmatrix} m_{11}u_{N-1} - u_{N-2} & m_{12}u_{N-1} \\ m_{21}u_{N-1} & m_{22}u_{N-1} - u_{N-2} \end{bmatrix}, \]  

(8.17)

with \( \chi = \frac{1}{2} Tr M \), \( u_N \) the Chebyshev polynomials of the second kind

\[ u_N(\chi) = \sin[(N + 1)\zeta]/\sin \zeta, \]  

(8.18)

and \( \zeta = \cos^{-1}\chi \) the Bloch phase of the periodic system [115], which is related to the eigenfunctions of M. In an infinite SL we have total reflection when \( \zeta \) is outside the range \((-1, 1)\).

For a single unit shown in Fig. 8.3(a) one can easily show that the full transfer matrix is given by

\[ M_T = M_d(-P)M(W, \varphi)M_d(P)M(W_s, \theta). \]  

(8.19)

We set \( L = W + W_s, \lambda_1^\pm = \theta \pm \beta_1, \lambda_2^\pm = \varphi \pm \beta_2, w = W/L \) and \( w_s = W_s/L \).

The spectrum of the structure is obtained from \( \cos(k_xL) = \chi = \frac{1}{2} Tr M \) [115, 116]. Inserting \( M_T \) from Eq. (8.19) we obtain the transcendental equation,

\[ \cos(k_x) = \cos(k_1w_s)\cos(k_2w) - \frac{E^2 - (k_y^2 - \beta^2/4)\cos(2P)}{k_2k_1} \sin(k_1w_s)\sin(k_2w). \]  

(8.20)

The solution of Eq. (20) gives the energy spectrum near the K point. The spectrum near the K’ point can be found by changing \( k_y \) to \(-k_y\). Note that the spectrum is symmetric under this change \( k \to -k \). For \( w = w_s \) the spectrum is also symmetric under the change \( k_y \to -k_y \). For \( w \neq w_s \) we have \( \langle A \rangle \neq 0 \) and the spectra near K and K’ are not individually symmetric about \( k_y \) however, we have \( E_K(k_x, k_y) = E_{K'}(k_x, -k_y) \).
8.3. KP MODEL: A SL OF MAGNETIC AND POTENTIAL δ-FUNCTION BARRIERS

Figure 8.4: ($k_y$, $k$) contour plot of the first conduction miniband with $W_s = 30$ nm, $P = \pi/2$, $\beta = 0$, and $a_s = 0$. Panels (a), (b), (c), and (d) are, respectively, for $W = 10$ nm, $W = 20$ nm, $W = 30$ nm, and $W = 40$ nm. The energy scale is $E_0 = \hbar v_F / (W + W_s)$.

8.3.2 A SL of potential barriers

The case of a pure potential SL ($\beta = 0$) was discussed before in Ref. [81]. Here we will derive analytical results in certain limiting cases which were not presented in Ref. [81]. Using a Taylor expansion for the dispersion relation in Eq. (8.20) we find

$$E^2 \approx k_x^2 + F^+ k_y^2,$$

(8.21)

with $F^+ = w^2 + w_s^2 + 2ww_s \cos(2P)$. Here, several cases are of interest:

1) $w + w_s = 1$, $\beta = 0$ and $P = \pi/4$. We have $k_1 = k_2$ and Eq. (8.20) reduces to

$$\cos(k_x) = \cos (k_1 w) \cos (k_1 w_s) - (E^2/k_1^2) \sin (k_1 w) \sin (k_1 w_s).$$

(8.22)

For $k, k_1 \to 0$, we obtain

$$k_x^2 = (w^2 + w_s^2) + 2E^2ww_s,$$

(8.23)

and consequently

$$E^2 = k_x^2 + (w^2 + w_s^2) k_y^2.$$ 

(8.24)

The velocity in the $y$ direction at the $K$ point is given by

$$v_y = \pm [w^2 + w_s^2]^{1/2},$$

(8.25)
and thus $1/\sqrt{2} \leq v_y/v_F < 1$. The minimum velocity in the $y$ direction is found for $w = w_s$, and the maximum one for $w \gg w_s$ or $w_s \gg w$.

2) $w + w_s = 1$, $\beta = 0$ and $P = \pi/2$. In this case the dispersion relation becomes,

$$\cos(k_x) = \cos(k_1) - 2k_y^2/k_1^2 \sin(k_1 w_s) \sin(k_1 w).$$

(8.26)

In the limiting case $k_1 \rightarrow 0$, Eq. (8.26) reduces to

$$E^2 = k_x^2 + k_y^2 \left( \frac{w_s - w}{w_s + w} \right)^2.$$  

(8.27)

The velocity at the $K$ point in the $y$ direction is given by

$$v_y = \pm \left| \frac{w_s - w}{w_s + w} \right|,$$

(8.28)

and thus there is perfect collimation only for $w = w_s$, i.e., for $v_y = 0$.

In Figs. 8.4(a)-(d) contour plots of the first miniband are shown for $W_s = 30$ nm and different values of $W$ shown in the caption. Notice that in Fig. 8.4(c) where we have a very good collimation along the $y$ direction that is very sensitive
8.3. KP MODEL: A SL OF MAGNETIC AND POTENTIAL $\delta$-FUNCTION BARRIERS

Figure 8.6: (a) 3D plot and (b) contour plot of the first energy band with $W = W_s = 30 \, \text{nm}$, $P = \pi/2$ and $B = 0$ (c)-(d) same as (a)-(b) but now for $\beta = 3.72$.

to the separation between the $\delta$-function barriers. As is evident from Figs. 8.4(c), 8.6(a) and 8.6(b) for $-0.25\pi/L < k_x < 0.25\pi/L$, the spectrum is almost linear and electron will be collimated if their wavelength is larger than $\lambda \sim 479 \, \text{nm}$ for $L = 60 \, \text{nm}$.

3) $w + w_s = 1$, $\beta = 0$ and $P = \pi$. In this limit Eq. (8.20) reduces to

$$\cos(k_x) = \cos(k_1),$$

then $k_1 = k_x + 2n\pi$ and $E_n^2(k_x, k_y) = (k_x + 2n\pi)^2 + k_y^2$. The first energy cone is located at the $K$ point while the second band is shifted by $2\pi$ in the $k_x$ direction.

### 8.3.3 Combined electric and magnetic SLs

Next we consider $\beta \neq 0$ and make a Taylor expansion in Eq. (8.20) to obtain the low-momentum dispersion relation

$$E - E_g \approx k_x^2 + \alpha(k_y - \lambda)^2.$$  (8.30)

Here $E_g$ is the band gap between electrons and holes, $\alpha = 1/2m^*$ the inverse of the effective mass ($\alpha = \partial^2 E/\partial k_y^2$), and $\lambda$ a shift in $k_y$ which depends on the choice of $w$ and $w_s$. For example, for $w = w_s$, $\lambda$ is zero because the vector potential area in regions 1 and 2 in Fig. 8.1(b) is the same and the two shifts cancel each other. But
for $w \neq w_s$ there will be a shift in the $k_y$ direction. For the special case $w = w_s$ we obtain the gap energy analytically,

$$E_g = \beta |\sin P|/2.$$  \hfill (8.31)

with $\Delta E = 2E_g$ the total energy gap.

Next, we consider two different strengths of the potential barriers:

**Case 1**) For $P = \pi/4$ the dispersion relation becomes

$$\cos(k) = \cos \left( k_1 w_s \right) \cos \left( k_2 w \right) - \left( E^2 / k_2 k_1 \right) \sin \left( k_1 w_s \right) \sin \left( k_2 w \right).$$  \hfill (8.32)

As shown in Fig. 8.5(c) in the presence of a magnetic SL a gap opens and the bound state along $k_y$ and around the gap position has a quadratic dependence on $k_y$ and consequently electrons and holes have a non zero mass. For $w \neq w_s$ we notice from Fig. 8.5(c) that the spectrum is no longer symmetric under the change $k_y \to -k_y$. This can be understood from the effective potential,

$$V_{eff} = \begin{cases} 
(k_y + \beta/2)^2, & \quad -w < x < 0 \\
(k_y - \beta/2)^2, & \quad 0 < x < w_s. 
\end{cases}$$  \hfill (8.33)

In Fig. 8.3(c) the effective potential is not symmetric for $k_y \to -k_y$ and also the vector potential in one period is not symmetric under the change $x \to -x$, i.e., we have $\langle A \rangle \neq 0$. As a consequence, the energy spectrum is no longer symmetric.
under the change $k_y \rightarrow -k_y$. Note that the velocity of the electron moving in the $y$ direction is not the same as for motion along the $x$ direction. The spectrum near the $K'$ point shows the opposite behavior. The spectra near the $K$ and $K'$ points are connected by $E_K(k_x, -k_y) = E_{K'}(k_x, k_y)$.

**Case 2**) $P = \pi/2$. Here we consider two different cases: 

a) $w = w_s$: in this case we expect to see collimation in the $k_y$ direction for $\beta = 0$, as shown in Figs. 8.6(a) and (b). Notice in passing an important feature in Fig. 8.6(a): instead of a Dirac point we have a Dirac line in agreement with Ref. [81]. For $\beta \neq 0$ an energy gap appears, see Figs. 8.6(c) and (d), and there is no longer collimation along the $k_y$ direction. 

b) $w \neq w_s$: in this case, as discussed in the previous section, there is no pure collimation in the $k_y$ direction and the electron velocity along this direction is non-zero. In the presence of a magnetic SL the center of the cone shifts in the $k_y$ direction but there is no gap and the cone of the second band remains in its previous position, see Figs. 8.7(a)-(d).
We complement our results by showing the DOS and the conductivities $\sigma_{xx}$ and $\sigma_{yy}$ for different potential strengths $P$ and by contrasting them with the results in the presence of a magnetic SL shown in Fig. 8.8. Notice that for $P = 3$ we obtain almost the DOS of pristine graphene, i.e., $D(E) \sim |E|$. When the magnetic SL is present an additional structure appears and the conductivity decreases. Notice also that $\sigma_{yy} \ll \sigma_{xx}$.

### 8.4 KP model with potential and magnetic SLs displaced with respect to each other

Next we consider the more general problem, see Fig. 8.1 for $a_s \neq 0$, when the potential and magnetic SLs are displaced with respect to each other. In this case the transfer matrix becomes

$$M_T = M_1 M_d(P) M_2 M_d(-P),$$

(8.34)
8.4. KP MODEL WITH POTENTIAL AND MAGNETIC SLS DISPLACED WITH RESPECT TO EACH OTHER

Figure 8.10: (a), (b): as in Figs. 8.4(a) and 8.4(b) for \( W = W_s = 30 \) nm, \( P = \pi/2 \) and \( \beta = 3.72 \), and \( a_s = 0.4W \). (c)-(d): the same as in (a)-(b) but for \( W = 20 \) nm, \( W_s = 40\) nm.

where \( M_1 = M(W-a_s, \varphi)M^\dagger(a_s, \varphi) \) and \( M_2 = M(W_s-a_s, \theta)M^\dagger(a_s, \theta) \). From these relations we can find the elements of \( M_1 \) and those of \( M_2 \). The spectrum is then obtained from \( \cos(k_x L) = \frac{1}{2} Tr \mathbf{M} \). Because the transcendental equation is too lengthy, we only present numerical results.

The numerical results are shown in Figs. 8.9, 8.10, and 8.11 for the different cases we discussed in the previous section. 3D plots of the first conduction and valence minbands and a contour plot of the first conduction minband are shown in Fig. 8.9 for \( P = \pi/4 \) and \( a_s = 0.42w \). Notice that the result for the first minband shows the same behavior as that without displacement, see Figs. 8.5(c)-(d). The symmetry with respect to \( k_y \) is broken and the electron velocity along \( k_y \) is different from that along \( -k_y \) (\( |v_{k_y}| \neq |v_{-k_y}| \)).

3D plots of the first conduction and valence minbands and contour plots of the first conduction band are shown in Fig. 8.10 for \( P = \pi/2 \) and two different cases, \( w = w_s \) and \( w \neq w_s \). For zero displacement \( (a_s = 0) \), \( w = w_s \), and in the presence of a magnetic SL there is no collimation, see Fig. 8.6(d), whereas there is one for a finite displacement \( a_s = 0.4w \), see Fig. 8.10(b) for small \( k \) only in the first minband. For \( w \neq w_s \) we see no collimation in Fig. 8.9(d). One difference for \( w \neq w_s \) and a finite displacement is that the center of the cone shifts along \( k_y \), see Figs. 8.10(c)-(d).

The numerical results for DOS and the conductivities \( \sigma_{xx} \) and \( \sigma_{yy} \), for different potential strengths \( P \) and \( a_s = 0.4w \), are shown in Fig. 8.11. As shown, for
8.5 Concluding remarks

We studied a combined magnetic and potential Kronig-Penney (KP) model for Dirac electrons in single layer-graphene with the relevant δ-function barriers alternating in sign. We obtained the electronic band structure, the DOS, and the diffusive conductivities perpendicular and parallel to the SL direction when the SL barriers are at the same place or displaced with respect to each other. In addition, we investigated electron collimation and how it changes when both δ-function barriers are present.
We found that the velocity $v_y$ for small $k$ in a potential SL, with $\beta = 0$ and $P = \pi/2$, is given by $v_y = \pm|((w - w_s)/(w + w_s))|$ and for $P = \pi/4$ by $v_y = \pm[w^2 + w_s^2]^{1/2}$. The collimation in case of a potential SL ($\beta = 0$) is very sensitive to the relative value of $w$ and $w_s$ and only for $w = w_s$ we have $v_y \approx 0$ for small $k$ (see Figs. 3(c) and 5(b)).

For $w \neq w_s$ the symmetry with respect to $k_y$ is broken and the spectrum is no longer symmetric for $k_y \rightarrow -k_y$. With combined magnetic and potential SLs a gap can be opened with size $\Delta E = \beta|\sin P|$ that is proportional to the height of the magnetic barriers and to a periodic function of the strength of the potential barriers. In the presence of a magnetic SL the collimation in the $y$ direction ceases to exist. Instead when the magnetic and potential SLs are shifted with respect to each other the collimation will return. The difference with the case without magnetic SL is that here we have also an energy gap induced by the magnetic field SL.
Quasi-bound states of Schrödinger and Dirac electrons in magnetic quantum dot

Abstract. The properties of a two-dimensional electron are investigated in the presence of a circular step magnetic field profile. Both electrons with parabolic dispersion as well as Dirac electrons with linear dispersion are studied. We found that in such a magnetic quantum dot no electrons can be confined. Nevertheless close to the Landau levels quasi-bound states can exist with a rather long life time.

9.1 Introduction

In this chapter we consider a finite size magnetic structure where the magnetic field is nonzero only in a finite region of space. Namely, we consider a model homogeneous magnetic field that is non-zero in a circle that we call the magnetic dot. This situation is the inverse of the one considered in Ref. [57] where a magnetic anti-dot was considered, as in Ref. [56] for the case of normal electrons, where the magnetic field is zero in a circular region and non-zero outside this region. Such a model system can be realized by having a magnetic vortex piercing the graphene layer or by overlaying graphene with type I superconductor with a circular hole placed in the perpendicular magnetic field. In order to reveal the peculiarities of the behavior of Dirac electrons in such magnetic dot we compare the result with those for standard electrons with parabolic dispersion law.

We show that it is impossible to confine 2D electrons in a magnetic dot in contrast to semi-infinite magnetic structures neither in the case of graphene nor in the case of the standard electron, and consequently, all Landau levels convert themselves into unbound states. Nevertheless, long living quasi-bound states can be present. We studied them using the local density of states technique applied previously for the investigation of electrically confined electrons [118].

The results of this chapter were published as:
9.2 Electron with parabolic energy dispersion

We assume that a homogeneous magnetic field \( B_0 \) is present in a circular area of radius \( r_0 \), while there is no magnetic field outside it, namely, \( B_0(r) = e_z B_0 \Theta(r_0 - r) \). The behavior of the electron is described by the stationary Schrödinger equation

\[
\{ H - E \} \Psi(r) = 0,
\]

with the Hamiltonian

\[
H = -\frac{1}{2} (\nabla + iA)^2.
\]

Because of the cylindric symmetry of the problem we choose the symmetric gauge for the vector potential defining its single azimuthal component as

\[
A_\phi(r) \equiv \frac{1}{2} \left\{ \begin{array}{ll}
  r, & r < r_0; \\
  r_0^2 / r, & r_0 < r.
\end{array} \right.
\]

This azimuthal component is shown in Fig. 9.1 together with the magnetic field profile.

In order to simplify the notations we use dimensionless variables, based on the magnetic field strength value \( B_0 \). Thus, the magnetic field \( B(r) \) is measured in \( B_0 \) units, all distances are measured in the unit of magnetic length \( l_B = \sqrt{\hbar/eB_0} \), energy and potential in \( \hbar \omega_c \) (\( \omega_c = eB_0/me \)), and vector potential in \( B_0 l_B \) units. In the case of electron moving at a GaAs/AlGaAs interface (\( m^* = 0.067 \)) and magnetic field of 1 T the unit of length is \( l_B = 250 \) nm, and the energy unit is 20 meV.
9.2. ELECTRON WITH PARABOLIC ENERGY DISPERSION

9.2.1 Solution of eigenvalue problem

The Schrödinger equation (9.1) in cylindric coordinates reads

\[
\left\{ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2}{\partial \varphi^2} + \frac{iA}{r} \frac{\partial}{\partial \varphi} - \frac{A^2}{r^2} + 2E \right\} \Psi = 0.
\] (9.4)

Substituting the wave function

\[
\Psi \equiv \Psi(r, \varphi) = e^{im \varphi} \psi(r)
\] (9.5)

we arrive at the radial equations

\[
\left\{ \frac{1}{r} d \frac{d}{dr} r d \frac{d}{dr} - \left( \frac{m}{r} + \frac{r^2}{2} \right)^2 + 2E \right\} \psi_I(r) = 0, \quad (9.6a)
\]

\[
\left\{ \frac{1}{r} d \frac{d}{dr} r d \frac{d}{dr} - \left( \frac{m + r_0^2/2}{r^2} \right)^2 + 2E \right\} \psi_{II}(r) = 0, \quad (9.6b)
\]

which have to be solved inside the dot (region I) and outside it (region II). The boundary conditions (the continuity of the wave function and its radial derivative) have to be satisfied at the dot border \((r = r_0)\).

The regular solution inside the dot can be expressed via the confluent hypergeometric function (Kummer function \(M(\alpha|\beta|z)\)):

\[
\psi_I(r) = A \psi_I(r) = A |m| e^{-r^2/4} \times M \left( |m| + \frac{1}{2} - E |m| + 1 \right), \quad (9.7)
\]

while the solution outside it is composed of two Bessel functions

\[
\psi_{II}(r) = B J_\nu(k r) + C Y_\nu(k r), \quad (9.8)
\]

where \(k = \sqrt{2E} \) is the momentum of the free electron (measured in \(l_B^{-1}\) units), and \(\nu = m + r_0^2/2\). Note both functions \((J_\nu \text{ and } Y_\nu)\) suit us, as they vanish in the limit \(r \to \infty\).

Thus, we have three constants \(A, B, \text{ and } C\). They can not be defined from the above mentioned two boundary conditions. That is why we have to conclude that there are no bound states, and consequently, a magnetic field in a finite region of the 2D plane can not confine the electron. However, quasi-bound states can be expected when the electron energy in the dot is close to the Landau levels with energy

\[
E_{n,m} = n + \frac{|m| + m + 1}{2} \quad (9.9)
\]
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Figure 9.2: The wave functions for $m = 0, r_0 = 5$: $E = 2.5$ – red solid curve, and $E = 2.8$ – dashed blue curve. The magnetic dot region is indicated by the shadowed colored rectangle.

(Here $n = 0, 1, \cdots$ and $m = 0, \pm 1, \cdots$) defined in the case of homogeneous magnetic field. Confirmation of this statement follows from Fig. 9.2, where the electron wave functions for two different energies are shown.

We see that in the case of $E = 2.5$ (red solid curve) which corresponds to the Landau level with $n = 2$ and $m = 0$ the wave function is large in the dot region (shown in Fig. 9.2 by the shadowed yellow rectangle), while for the case of energy $E = 2.8$, which does not coincide with any Landau level energy, it does not have any appreciable large value inside the dot, and actually does not differ much from the wave function for a free electron calculated in cylindric coordinates.

9.2.2 Local density of states

Next we will look for possible long living quasi-stationary states in the magnetic dot. In principle such quasi-bound (or quasi-stationary) states have to be described by the solution of the time dependent Schrödinger equation which is much more complicated as compared with the standard eigenvalue problem. There are, however, several alternative approaches which enable us to investigate properties of quasi-bound states by stationary means. We follow the method presented in detail in Ref. [118], and calculate the local density of states. The basic idea is to confine the electron in a large region of finite radius $R$, where its wave function obeys the zero boundary condition at the border ($r = R$) and treat the problem as a stationary one. A measurement that probes quantum dot properties, say, measuring of the tunnelling current directed perpendicular to the dot with STM, or power absorp-
9.2. ELECTRON WITH PARABOLIC ENERGY DISPERSION

tion in near field infrared spectroscopy, has to depend on the averaged value of the electron wave function in the dot. Therefore we introduce the integral

$$\mathcal{I}(E) = 2\pi \int_0^\infty r dr F(r)|\Psi(r)|^2,$$

(9.10)

which depends on the electron wave function, and actually is proportional to the so called local density of states. The aperture function $F(r)$ characterizes the interaction of the electron with the measuring probe.

This integral is sensitive to the probability to find the electron in the dot, and in the case of a quasi-bound state it will exhibit a peak corresponding to the energy of this state. The width of the peak is related to the inverse of the life time of this quasi-stationary state.

For the sake of determinacy we use the aperture function of a gaussian:

$$F(r) = br^2_0 e^{-br^2}, \quad b = r_0^{-2} \ln 10,$$

(9.11)

which corresponds to the probability to find the electron in the dot area $\pi r_0^2$. In the case of larger $b$ value instead of the local density of states we obtain the squared wave function value in the center of the dot, while in the case of smaller $b$ value the peculiarities of the dot are washed out.

The solution of the Schrödinger equation (9.6) given by Eqs. (9.7) and (9.8) has to satisfy the following boundary conditions:

$$\psi_I(r_0) = \psi_{II}(r_0),$$

(9.12a)

$$\psi_{I,r}(r_0) = \psi_{II,r}(r_0),$$

(9.12b)

$$\psi_{II}(R) = 0,$$

(9.12c)

which converts our problem into an eigenvalue problem. Here and further the subscript $r$ means the derivative over $r$.

At the end, we are interested in the limiting case $R \to \infty$. Therefore, in the last of Eqs. (9.12) we replace the Bessel functions by their asymptotic, namely, we have

$$B \cos(kR - \varphi_m) + C \sin(kR - \varphi_m) = 0,$$

$$\varphi_m = \pi \left\{ m + (r_0^2 + 1)/2 \right\}/2,$$

(9.13)

instead of Eq. (9.12c).

Postponing till later the proper wave function normalization we assume that $B = \cos \Phi$ and $C = \sin \Phi$ and rewrite the above equation as

$$\cos(kR - \varphi_m - \Phi) = 0.$$

(9.14)
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This equation shows that the eigenvalues of the considered problem are approximately separated by $\Delta k = \pi / R$, and reduce to a continuum spectrum in the limit $R \to \infty$. Constructing some averaged description which is valid when calculating the local density of states, we replace Eq. (9.12c) by the following one:

$$B^2 + C^2 = 1.$$ (9.15)

Now solving it together with Eqs. (9.12a,b) we obtain three constants:

$$A = -\frac{2}{\pi r_0} W, \quad B = W Q, \quad C = -W P,$$ (9.16)

with

$$P = J_{\nu f} - J_{\nu r} f, \quad Q = Y_{\nu f} - Y_{\nu r} f,$$ (9.17a)

$$W = \left( P^2 + Q^2 \right)^{-1/2}.$$ (9.17b)

The obtained constants enable us to calculate the integral (9.10).

In order to convert the above integral into the local density of states we have to multiply it by two additional constants. One of them is the wave function normalization factor $N$, which can be estimated calculating the integral of the squared wave function in the limit of large radius $R$. The replacement of the Bessel functions by their asymptotic immediately leads to $N = k/2R$. The second one is a consequence of the replacement of the summation over the discrete eigenvalues by the integration over energy, which is given by the factor $R/\pi k$. Together they give $1/2\pi$, which results into definition of the local density of states

$$\rho(E) = \frac{1}{2\pi} \mathcal{I}(E).$$ (9.18)

9.2.3 Numerical results

We solved numerically Eqs. (9.17). Inserting the obtained results into (9.16), and later in Eqs. (9.7) and (9.8) we obtained the wave function what enabled us to calculate the integral (9.10), and finally the local density of states (9.18).

A typical result for the local density of states as a function of electron energy is shown in Fig. 9.3. We clearly see peaks close to the energies of the Landau levels (9.9) calculated for the case of a homogeneous magnetic field. These peaks are broadened indicating that they are not really bound states in the magnetic dot. The broadening is larger for higher energy peaks.
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Figure 9.3: The local density of states for $m = 0$ and $r_0 = 3$ shown by the solid red curve. The same density calculated for a free electron according to Eq. (9.20) is shown by the blue dashed curve.

The next thing which also is seen in Fig. 9.3 is a decreasing background with energy. This background is due to the states of the free electron in the absence of the magnetic dot. To justify this statement we made the same averaging (over circle of radius $r_0$) with the same gaussian aperture function (9.11) of the radial component of the free electron wave function (when there is no magnetic dot). This function reads

$$\psi_{\text{free}}(r) = J_m(kr)$$  \hspace{1cm} (9.19)

and is valid in the whole 2D plane. Inserting this function into integral (9.10) and later in Eq. (9.18) and using Tables of integrals [100] we obtain the local density of states for a free electron

$$\rho_{\text{free}}(E) = \frac{r_0^2}{2} e^{-E/b} I_m(E/b),$$  \hspace{1cm} (9.20)

where $I_m(x)$ stands for the modified Bessel function of the first kind. This local density of free electron in the case of $m = 0$ is shown in the same Fig. 9.3 by the blue dashed curve. Comparing these two curves we clearly see how increasing the electron energy we reduce the influence of the magnetic dot on the electron behavior, and the local density of states converts itself gradually into the free electron one.

We fitted the peaks in the density of states by Lorentzian functions $a_n\gamma_n\{(E - E_n)^2 + \gamma_n^2\}$ defining three parameters for any of them: the position $E_n$, its broad-
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ening $\gamma_n$, and the amplitude $a_n$. Two of them (the position and broadening) are shown in Figs. 9.4 and 9.5 for different orbital momenta as functions of the radius of the dot $r_0$. The position of the quasi-bound states $E_n$ are shown by the red solid curves while the broadening of the peaks is indicated by the shadowed areas limited by the $E_n \pm \gamma_n$ curves.

![Figure 9.4: Quasi-bound states with orbital momentum $m = 0$. The energies of these states are given by red solid curves and the widths (i.e. the inverse of the life time) by shadowed regions. The Landau levels are indicated by blue dashed lines.](image)

Notice that the levels to the right of the green dotted curve are extremely narrow and their position coincides with the Landau levels (9.9) shown by the blue dashed horizontal lines. In fact this means that almost all electron wave function is located in the magnetic dot (using the classical description language we may say that the electron rotates along the Larmor circle inside the dot) and it does not touch the border of the magnetic dot. When the dot radius $r_0$ becomes smaller the Larmor circle touches the dot border and tunnelling of the electron outside the dot starts which broadens the level. The partial penetration of the wave function outside the dot leads to a lowering of the quasi-bound state energy as well. The raising of this energy for small $r_0$ values is caused by the large asymmetry of the peak where actually the approximate replacement of the peak by a Lorentzian type function is no longer valid. This picture is more or less the same for all positive $m$ values (compare Figs. 9.4 and 9.5). The difference is that for larger $m$ values the levels start at higher energies what is in agreement with the expression for Landau levels (9.9).
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The picture for negative $m$ values is different as shown in Fig. 9.6. All of them belong to the same Landau level energy which is an expression of the degeneracy of the Landau level. We see that with decreasing radius of the dot $r_0$ the levels with different $m$ disappear step by step, the ones with smaller absolute $m$ values disappear later. This is in agreement with the fact that the larger the $|m|$ value the larger the radius of the electron trajectory, and the electron wave function is closer to the dot edge.

The increase of the peak broadening at small $r_0$ values is so steep that it is worth to divide all the peaks into two classes as shown in the above figures by the green dotted curves. The levels on the left side of these curves belong to essentially broadened quasi-bound states, while those on the right side from the experimental point of view can hardly be distinguished from the real bound states.

One can crudely estimate the position of this dividing curve comparing the approximate dimensions of the electron wave function calculated in the case of a homogeneous magnetic field (which actually coincides with function (9.7)) with the magnetic dot radius $r_0$. A more accurate estimation can be obtained solving the stationary Schrödinger equation for complex energy eigenvalues as was described in Ref. [119]. We draw these dividing curves in Figs. 9.4-9.6 using this technique which is sketched in the following section.
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Figure 9.6: The lowest quasi-bound state with \( n = 0 \) and different negative \( m \) values. The vertical dotted green lines are the analog of the dotted curve in Figs. 9.4 and 9.5, separating the weakly broadened states from those with small lifetime.

9.2.4 Complex energy technique

According to Ref. [119] the lifetime of the quasi-bound state, or the trapping time of the electron in the quantum dot can be estimated solving the time-independent Schrödinger equation and applying boundary conditions of the outgoing waves at the sharp dot border.

In our case this technique reduces to connecting the wave function (9.7) defined in the dot with the outgoing electron wave function outside it, which is given by the Hankel function of the first kind,

\[
\psi_{\text{out}}(r) = H^{(1)}_\nu(kr) = J_\nu(kr) + iY_\nu(kr) \tag{9.21}
\]

with

\[
\nu = m + r_0^2/2. \tag{9.22}
\]

Applying the boundary conditions for these wave functions and their derivatives we obtain the following equation:

\[
f_r(r_0)H(kr_0) - f(r)H_r(kr_0) = 0, \tag{9.23}
\]

where for the sake of simplicity we omitted the indexes of the Hankel functions. The indexes which are only left indicates the derivative over the coordinate \( r \). This equation has to be solved for a complex energy (or complex \( k \)), the imaginary part of the energy gives the inverse of the lifetime.
For finding the dotted curves in Figs. 9.4-9.6 separating the quasi-bound and nearly bound states it is enough to solve the above equation by means of a perturbation expansion in terms of the momentum difference $\Delta k = k - k_0$ where $k_0 = \sqrt{2E_{n,m}}$ with energy $E_{n,m}$ of the unperturbed Landau level. Limiting ourselves to first order in $\Delta k$ we arrive at the following expression:

$$\Delta k = \frac{H_{rf} - H_{fr}}{H_{fr,k} + H_{kfr} - H_{fr,k}}. \quad (9.24)$$

All functions and their derivatives over $r$ and $k$ have to be calculated at $r = r_0$ and $k = k_0$.

Now introducing the energy deviation from the Landau level energy

$$\Delta E = E - E_{n,m} \approx k_0 \Delta k, \quad (9.25)$$

taking its imaginary part and equating it to $10^{-2}$ (it is expected that a smaller broadening can hardly be revealed experimentally) we obtained the points connected by the green dotted curve in Figs. 9.4-9.6 separating the quasi-bound states from nearly bound states.

### 9.3 Dirac electron in graphene

Now we repeat the above calculation for the magnetic dot applying it to the case of a Dirac electron in graphene, where the low-energy quasi-particles (electrons and holes) are described by the following dimensionless Dirac-like Hamiltonian:

$$H = \sigma \left( -i\nabla + A \right). \quad (9.26)$$

Here, $\sigma = \{\sigma_x, \sigma_y\}$ stands for the $2 \times 2$ Pauli matrices. The units are based on the magnetic field strength $B_0$ and they are the same as in previous section, except the unit of energy which now is $v_F \hbar / l_B$ with the Fermi velocity $v_F = 10^8$ cm s$^{-1}$. In the case of a 1 T magnetic field this energy unit is 2.6 meV. The vector potential is given by Eq. (9.3).

### 9.3.1 Solution of eigenvalue problem

The approach is based on the same stationary Schrödinger equation (9.1) but now with the matrix Hamiltonian (9.26), which results into a set of two differential equations. Assuming the wave function of the following form:

$$\Psi = e^{im\varphi} \begin{pmatrix} a(r) \\ ie^{i\varphi} b(r) \end{pmatrix}, \quad (9.27)$$

## 9.3. DIRAC ELECTRON IN GRAPHENE
we arrive at a set of two equations for the radial wave function components

\[
\begin{align*}
\left\{ \frac{d}{dr} + A(r) + \frac{m+1}{r} \right\} b &= E a, \\
- \left\{ \frac{d}{dr} - A(r) - \frac{m}{r} \right\} a &= E b,
\end{align*}
\]

which has to be solved in the two regions (I in the dot, and II outside it). We require the continuity of the obtained components at the dot border \(r_0\)

\[
a_I(r_0) = a_{II}(r_0), \quad b_I(r_0) = b_{II}(r_0).
\]

Instead of solving these first order differential equations it is more convenient to convert them into second order differential equations for a single component, say for component \(b\)

\[
\begin{align*}
\left\{ \frac{1}{r} \frac{d}{dr} \frac{d}{dr} - \frac{(m+1)^2}{r^2} - \frac{r^2}{4} + \frac{E^2 - m}{r^2} \right\} b_I &= 0, \\
\left\{ \frac{1}{r} \frac{d}{dr} \frac{d}{dr} + \frac{E^2 - (m + 1 + r_0^2/2)^2}{r^2} \right\} b_{II} &= 0.
\end{align*}
\]

In contrast to the electrical quantum dot case which was considered in Ref. [118] now the effective potential in Eqs. (9.28) is a continuous function at the dot border. For this reason the boundary conditions (9.29) are equivalent to

\[
b_I(r_0) = b_{II}(r_0), \quad b_{I,r}(r_0) = b_{II,r}(r_0).
\]

These boundary conditions are identical to those for the previous Schrödinger electron case (9.12). It enables us to use the full analogy with the previous case. Taking this analogy into account we have for the solution in the two regions

\[
b_I(r) = Af(r) = Ar^{m+1}e^{-r^2/4}M(a_0|c_0|/2), \quad b_{II}(r) = BJ_\nu(kr) + CY_\nu(kr).
\]

where \(k = |E|, \quad a_0 = (|m + 1| + m + 1 - E^2)/2, \quad \nu = m + 1 + r_0^2/2, \) and \(c_0 = |m + 1| + 1.\) The expressions for the other wave function component \(a(r)\) follow directly from Eq. (9.28a):

\[
\begin{align*}
a_I(r) &= \frac{A}{E} r^{m+1}e^{-r^2/4} \\
&\times \left\{ \frac{d}{dr} + \frac{|m + 1| + m + 1}{r} \right\} M(a_0|c_0|/2), \\
a_{II}(r) &= BJ_{\nu-1}(kr) + CY_{\nu-1}(kr).
\end{align*}
\]
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Figure 9.7: The wave function components: \( a \) – dashed blue curve, and \( b \) – red solid curve, for \( m = 0 \), dot radius \( r_0 = 5 \) and two energy values: \( E = 1.932 \) – upper plot, \( E = 2.470 \) – lower plot.

The wave function components obtained in the above way are illustrated in Fig. 9.7 for two different values of the energy. We see the same tendency. When the energy is close to the Landau level energy of the Dirac electron in a homogeneous magnetic field,

\[
E_{n,m} = \pm \sqrt{2n + |m + 1| + m + 1},
\]

(9.34)

(see the lower plot of Fig. 9.7 where the energy is close to the Landau level with \( m = 0, n = 2 \)) we see a clear accumulation of the wave function components in the dot, what indicates a quasi-bound state.

9.3.2 Local density of states

Developing further the analogy of Eq. (9.30) with the considered previously case we calculated the local density of states using Eqs. (9.17), (9.16) and (9.10). Because we have now a wave function with two components, Eq. (9.10) is modified into

\[
\mathcal{I}(E) = 2\pi \int_0^\infty r dr F(r) \left\{|a(r)|^2 + |b(r)|^2\right\}.
\]

(9.35)

Now the normalization factor is \( N = k/4R \) (due to the two wave function components), and the factor responsible for the change of the summation over discrete eigenvalues into an integral over the electron energy is \( R/\pi \). Thus, the local density of states in the case of a Dirac electron becomes

\[
\rho(E) = \frac{|E|}{2} \int_0^\infty r dr f(r) \left\{|a(r)|^2 + |b(r)|^2\right\}.
\]

(9.36)
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In the case of free Dirac electrons (when there is no magnetic dot) the wave function components read

\[ a_{\text{free}} = J_m(kr), \quad b_{\text{free}} = J_{m+1}(kr), \quad (9.37) \]

what leads to the following expression of the local density of states for a free electron:

\[ \rho_{\text{free}}(E) = \frac{|E|r_0^2}{4} e^{-E^2/2b} \left\{ I_m(E^2/2b) + I_{m+1}(E^2/2b) \right\}. \quad (9.38) \]

9.3.3 Numerical results

The typical local density of states calculated for \( m = 0 \) and \( r_0 = 3 \) is shown in Fig. 9.8 for positive energies. Two differences with respect to standard electrons can clearly be noticed. First, in the case of the Dirac electron the spectrum is symmetric with respect to energy inversion \( (E \rightarrow -E) \) due to the equivalence of electrons and holes. Thus the plot in Fig. 9.8 has to be supplemented by the same curves for negative energies. Second, comparing the density of states for Dirac electron with the same curve for the Schrödinger one (see Fig. 9.3) we see that there are more peaks. This can be explained by the more dense Landau level spectrum in the case of Dirac electrons (9.34) for the large quantum number values as compared with these for the previous case (9.9).
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Figure 9.9: Quasi-bound states with orbital momentum $m = 0$ for the Dirac electron in the magnetic dot. The energy of these states are given by red solid curves and its width (i.e. the inverse of the life-time) by the shadowed regions. The Landau levels are indicated by blue dashed lines.

As before we fit the peaks by Lorentz type curves what leads to the broadened levels displayed in Figs. 9.9 and 9.10.

We see that the levels with $m = -1$ start at lowest energies what is just the consequence of chosen definition of radial wave function components (9.27).

The green dotted curves divide the region of broadened quasi-bound states from the region where the states have a very small broadening. These curves were obtained in the same way as it was done in section 9.2.4 for the case of Schrödinger electron, namely, applying the complex energy eigenvalue technique. In the case of the Dirac electron it leads to the following imaginary energy part:

$$\Delta = \frac{H_{\nu-1}b - H_{\nu}a}{H_0 a_T + H_{\nu}a - H_{\nu-1}b_T - H_{\nu-1}b}.$$  \hspace{1cm} (9.39)

The above mentioned dotted green line corresponds to $\delta = 3 \cdot 10^{-3}$. Note we chose it three times smaller than in Figs. 9.4-9.6 what causes us to conclude that between the local density of states technique and complex energy eigenvalue method one can expect only qualitative agreement.

There is one more interesting point — the zero energy state which is shown in Fig. 9.10 by thick red line along the $x$-axis. Its behavior differs essentially from all other states. That is why it needs some special attention which is presented in the
next subsection.

9.3.4 Zero energy state

Now we check whether the Dirac electron has a zero energy state in the magnetic dot. In this case instead of Eqs. (9.28) we have to solve the following two equations for the radial components of the electron wave function:

\[
\begin{align*}
\left\{ \frac{d}{dr} + A(r) + \frac{m + 1}{r} \right\} b &= 0, \quad (9.40a) \\
\left\{ \frac{d}{dr} - A(r) - \frac{m}{r} \right\} a &= 0. \quad (9.40b)
\end{align*}
\]

These are uncoupled differential equations of the first order, and their solution can be found by a straightforward integration. The solution has the following asymptotic behavior:

\[
\ln a(r) = \int dr \left\{ A(r) + \frac{m}{r} \right\}
\sim \begin{cases} 
  m \ln r + r^2/4, & r \to 0; \\
  (m + r_0^2/2) \ln r, & r \to \infty,
\end{cases}
\quad (9.41)
\]

Figure 9.10: The same as Fig. 9.4 but now for \( m = -1 \).
9.4. CONCLUSIONS

and

\[
\ln b(r) = - \int dr \left\{ A(r) + \frac{m + 1}{r} \right\}
\]

\[
\sim \begin{cases} 
-(m + 1) \ln r - r^2/4, & r \to 0; \\
-(m + 1 + r^2_0/2) \ln r, & r \to \infty,
\end{cases}
\]

or

\[
a(r) \sim \begin{cases} 
 r^m \exp(r^2/4), & r \to 0; \\
 r^{m+r^2_0/2}, & r \to \infty,
\end{cases}
\]

and

\[
b(r) \sim \begin{cases} 
r^{-m-1} \exp(-r^2/4), & r \to 0; \\
r^{-(m+1+r^2_0/2)}, & r \to \infty.
\end{cases}
\]

In order to have the wave function with finite norm two boundary conditions have to be satisfied. First, the function should behave like \( r^\alpha \) (\( \alpha \geq 0 \)) when \( r \to 0 \), and second, it should behave like \( r^{-\alpha} \) (\( \alpha \leq -1 \)) when \( r \to \infty \).

For the \( a \) component the above conditions reduce to the requirements \( m \geq 0 \) and \( m + r^2_0/2 \leq -1 \), which can not be satisfied simultaneously. Consequently, we have to assume that \( a = 0 \).

In the case of component \( b \) the conditions read

\[
-r^2_0/2 \leq m \leq -1,
\]

from which it follows that if \( r^2_0/2 \geq 1 \) there are always some negative \( m \) values for which a zero energy state exists. When the radius of the dot decreases this interval becomes smaller, and the zero energy states vanish one by one. Finally, at \( r^2_0/2 < 1 \) all of them disappear.

Such essential difference between the bound zero energy level and all other quasi-bound levels is caused by the fact, that the wave function of the state with zero energy is real. Consequently, the electron in this state has no velocity, and as a result there is no tunnelling of this electron outside the dot. Unfortunately, the absence of any non zero electron velocity makes it impossible to reveal this state in transport measurements, but maybe it can reveal itself through the statistic properties of the magnetic dot.

9.4 Conclusions

We considered the eigenvalue problem of a model quantum magnetic dot where the homogeneous magnetic field perpendicular to the 2D electron motion plane is
created only in a finite region — in a circle of radius $r_0$. We showed that such a magnetic field fails to confine electrons both for the standard parabolic dispersion law or the ultra relativistic linear dispersion law for Dirac electrons in graphene. Although in such a magnetic dot no confined states are found, quasi-bound states with a finite lifetime are present.

An analysis of the quasi-bound states for the Schrödinger and Dirac electron was performed by means of the local density of states, and the position and width of the resonance peaks (the analogs of the quasi-stationary states), on the dot radius (or the strength of the magnetic field) were calculated.

The broadening of these peaks (the inverse lifetime of the quasi-bound state) is mainly caused by the touching of the quantum dot border by the electron wave function tail. Due to the exponential character of this tail there exist a rather sharp border between broadened quasi-bound states and those which can be considered as nearly bound ones. This border was found by applying the complex energy eigenvalue method which is shown to be in qualitative agreement with the results obtained from the local density of states technique.

It is shown that the difference of the quasi-bound states in the magnetic dot between the Schrödinger and Dirac electrons is only in the energies of these states which is a consequence of the different energies of the corresponding Landau levels.

There is a single exception: in the case of Dirac electrons there exists a zero energy bound state for negative values of the angular momentum (the momentum which is opposite to the direction of the classical electron rotation along the Larmor circle). When the dot radius $r_0$ (or the magnetic field strength) decreases the degeneracy of this zero energy level decreases while all other quasi-bound states disappear smoothly via their broadening.
Graphene in inhomogeneous magnetic fields: Bound, quasi-bound and scattering states

Abstract. In this chapter magnetic dot and magnetic ring structures and combinations of both are considered. The corresponding spectra are studied as a function of the radii, the strengths of the inhomogeneous magnetic field and of a uniform background field, the strength of an electrostatic barrier and the angular momentum quantum number. In the absence of an external magnetic field we have only long-lived quasi-bound and scattering states and we assess their influence on the density of states. In addition, we consider electron scattering by a magnetic dot such that the average $B$ vanishes, and show that the Hall and longitudinal resistivities oscillate as function of the electron energy. Shape structures in these resistivities are a consequence of the presence of quasi-bound states.

10.1 Introduction

We consider finite-size magnetic structures in which the magnetic field is inhomogeneous and treat both bound, quasi-bound states and scattering with emphasis on the latter. We do that for a magnetic dot and a ring in the presence or the absence of a tunable external homogeneous magnetic field. In addition, we study a specific profile in which a dot, in a field $-B$, is surrounded by a ring, of finite width, in a field $B$ and evaluate the quasi-bound states. Such inhomogeneous magnetic field profiles can be realized by having a magnetic vortex piercing the graphene layer or by covering graphene with a type I superconductor with a circular hole or annulus placed in a perpendicular magnetic field. Another way is by deforming the

*The results of this chapter were published as:
lattice locally; this results in a local strain which in graphene can induce an effective inhomogeneous magnetic field [69, 108]. We also include in the calculation electrostatic potential barriers.

In chapter 9 it was shown that it is impossible to confine 2D electrons in a magnetic dot, in contrast to semi-infinite magnetic structures, since all Landau levels (LLs) convert themselves into unbound states. Nevertheless, long-living, quasi-bound states can be present [120]. In view of that we carry out a similar study but for more complex magnetic field profiles, in the presence or absence of an external magnetic field, and show that in its presence bound states do exist. We focus on the behavior of the quasi-bound states and show that they affect various properties, e.g., the density of states and the magneto and Hall resistivity. In particular, we consider electron scattering by a magnetic dot with zero average $B$ vanishes and evaluate the Hall and longitudinal resistivities as functions of the electron energy.

## 10.2 Basic formalism

We consider electrons in graphene in a perpendicular magnetic field $B$. The relevant eigenvalue problem is

$$\{H - E\} \Psi(r) = 0 \quad (10.1)$$

with the Hamiltonian for a Dirac electron given by

$$H = v_F \sigma \cdot (p + eA) = \begin{pmatrix} 0 & -ip_+ + A_- \\ -ip_+ + A_+ & 0 \end{pmatrix}, \quad (10.2)$$

where $p_\pm = \partial/\partial x \pm i \partial/\partial y$ and $A_\pm = A_x \pm iA_y$; $A$ is the vector potential and $v_F$ the Fermi velocity. To simplify the notation we introduce the dimensionless variables $B \rightarrow B_0B, \quad A \rightarrow B_0RA, \quad t \rightarrow tR/v_F, \quad r \rightarrow Rr, \quad v \rightarrow v_Fv, \quad E \rightarrow E_0E, \quad E_0 = hv_F/R, \quad \gamma_i = eB_iR^2/2h$. $R$ is the radius of a dot, and $E$ the energy.

In view of the geometry of the profiles we consider polar coordinates. This is accomplished by the relations $x \pm iy = re^{\pm i\varphi}, \quad p_\pm = e^{\pm i\varphi}[\partial/\partial r \pm (i/r)\partial/\partial \varphi]$. We look for solutions that are periodic in the angle $\varphi$. Then we can write the two-component wave function $\Psi$ in the form

$$\Psi = \begin{pmatrix} \psi_1(r, \varphi) \\ \psi_2(r, \varphi) \end{pmatrix} = e^{im\varphi} \begin{pmatrix} a(r) \\ ie^{i\varphi} b(r) \end{pmatrix}, \quad (10.3)$$

with $m = \cdots, -2, -1, 0, 1, 2, \cdots$. Combining Eqs. (10.1) and (10.3) we find that the components $a(r)$ and $b(r)$ must satisfy this coupled, first-order
10.2. BASIC FORMALISM

differential equations
\[
\begin{align*}
\{d/dr + g(r) + (m + 1)/r\} b(r) &= E a(r), \\
\{d/dr - g(r) - m/r\} a(r) &= E b(r),
\end{align*}
\] (10.4a, 10.4b)

where \(g(r) = \gamma_i r + s_i/r\). It is convenient to transform Eqs. (4) to a single, second-order equation. We readily find that the equation for the component \(b(r)\) reads
\[
\left\{ \frac{1}{r} d^2 r - \frac{d}{dr} + \left[ -\gamma_i^2 r^2 - P_i^2 / r^2 + Q_i^2 \right] \right\} b(r) = 0,
\] (10.5)

with \(P_i^2 = (s_i + m + 1)^2\) and \(Q_i^2 = E^2 - 2\gamma_i [s_i - (m + 1)]\). A similar equation is obtained for the component \(a(r)\).

The solution of Eq. (10.5) is
\[
b(r) = r |P_i| e^{-|\gamma_i|r^2/2} \{ A_i M (\alpha_i, \beta_i, z_i) + B_i U (\alpha_i, \beta_i, z_i) \},
\] (10.6)

with \(\alpha_i = (|P_i| + 1)/2 - Q_i^2/4|\gamma_i|, \beta_i = |P_i| + 1, \text{ and } z_i = |\gamma_i|r^2\). Here \(M(\ldots)\) and \(U(\ldots)\) are the confluent hypergeometric functions. From Eq. (10.4a) we obtain
\[
a(r) = \frac{1}{E} \left[ 2|\gamma_i|r \frac{d}{dz_i} + \left( (\gamma_i - |\gamma_i|)r + 2|P_i|/r \right) \right] b(r).
\] (10.7)

10.2.1 Homogeneous magnetic field

The solution for the component \(a(r)\) in a homogenous field \(B\), with taking the unit of length \(R = \ell_B = (\hbar/eB)^{1/2}\) equal to the magnetic length \((\gamma_i = 1/2\) and \(E_0 = \hbar v_F/\ell_B\)) and \(s_i = 0\), can be written in terms of the confluent hypergeometric function \(M(\ldots)\) as
\[
a_\ldots (r) = Ar^m e^{-r^2/4}
\times M \left( (|m| + m + 2 - E^2)/2, |m| + 1, r^2/2 \right).
\] (10.8)

This expression enables us to obtain bound states in the case of a homogeneous magnetic field. Indeed, in this case the above solution is finite in all regions provided the first argument of the function \(M(\ldots)\) is a negative integer or zero, namely, \((|m| + m + 2 - E^2)/2 = -n, n = 0, 1, 2, \cdots\). This gives the energy \(E \equiv E_{nm}\)
\[
E_{nm} = \sqrt{2n + |m| + m + 2}.
\] (10.9)

Thus, we have the standard expression for the LLs of a Dirac electron starting from the level
\[
E_{00} = \sqrt{2}.
\] (10.10)
This is not the lowest LL. Thus, let us consider the equation for the component \( b(r) \). Its solution reads
\[
b(r) = A r^{\mid m+1 \mid} e^{-r^2/4} \times M \left( (\mid m + 1 \mid + m + 1 - E^2)/2, \mid m + 1 \mid + 1, r^2/2 \right).
\] (10.11)
Setting the first argument of \( M \) equal to a negative integer \(-n\) gives
\[
E_{nm} = \sqrt{2n + \mid m + 1 \mid + m + 1}
\] (10.12)
This expression for the LLs coincides with that given by Eq. (10.9) except for the lowest level which is
\[
E_{0,-1} = 0
\] (10.13)
It corresponds to the known fact that the lowest LL for a Dirac electron has half the degeneracy of the other LLs. In the case of a magnetic ring, which we will consider below, we expect that bound states will appear close to the positions of the LLs given by Eq. (10.12).

Figure 10.1: Two configurations of a magnetic dot, created by a field \( B_1 \), in an external magnetic field \( B_2 \) and the corresponding magnetic field (black lines) and vector potential (red lines) profiles.

10.3 Bound states

10.3.1 Magnetic dot

Quasi-bound states in a magnetic dot were treated before in Ref. [120]. Here we focus on the bound states that occur when the dot is placed in a uniform magnetic
10.3. BOUND STATES

field; generalizes the results of Ref. [57] valid for zero background field. The situation is depicted in Fig. 10.1 and the corresponding vector potential is given by

\[
A(r) = \begin{cases} 
\gamma_1 r; & 0 < r < 1, \\
\gamma_2 r + (\gamma_1 - \gamma_2)/r; & r > 1,
\end{cases}
\]  

(10.14)

where \( r \) is the radial coordinate in units of \( R \), the dot radius. Then the solutions for \( b(r) \) in the two regions, inside the dot \( r < 1 \) and outside it \( r > 1 \), are

\[
b(r) = \begin{cases} 
Ar^{|p_1|}e^{-|\gamma_1|r^2/2}M(\alpha_1, \beta_1, z_1); & 0 < r < 1, \\
Br^{|p_2|}e^{-|\gamma_2|r^2/2}U(\alpha_2, \beta_2, z_2); & r > 1.
\end{cases}
\]  

(10.15)

Those for the component \( a(r) \) can be found from Eq. (10.4).

To calculate the bound states we match the wave functions at \( r = 1 \). Then we obtain the energy states by satisfying the boundary condition at \( r = 1 \). This leads to

\[
[b^+(r)a^-(r) - b^-(r)a^+(r)]_{r=1} = 0,
\]  

(10.16)

where \( +(-) \) refers to the region inside (outside) the dot. The numerical results

Figure 10.2: (a) Energy spectrum versus external magnetic field \( B_{\text{ext}} \) for the circular magnetic field profile shown in the inset with \( B_0 = -2T \), \( R = 50 \) nm and \(-1 \leq m \leq 1\). as function of the background magnetic field \( B_{\text{ext}} \) are shown in Fig. 10.2 for three different values of the angular momentum \( m \). Notice that i) for \( |B_{\text{ext}}| \gg |B_0| \) the usual LLs of electrons in graphene are recovered, and ii) for \( B_{\text{ext}} \to 0 \) there are no bound states as discussed previously in Ref. [120]. In Fig. 10.3(a) the energy
states are plotted as a function of the dot radius with the magnetic field inside the dot chosen as $B_1 = -B_2/2$, and the ratio of the corresponding LLs inside and outside the dot being $E_{out}^{LL} = \sqrt{2}E_{in}^{LL}$. This means that for quantum numbers $n_{out} = 2n_{in}$ the LLs inside and outside the dot have the same values. Since the magnetic field inside and outside the dot have opposite sign we have bonding and anti-bonding states [121] as is clearly apparent for $n = 2$ in Fig. 10.3(a). We can also calculate the angular current using $j_{x,y} = v_F \Psi(10.17)$.
10.3. BOUND STATES

Figure 10.4: (a) Energy spectrum for the magnetic field profile shown in Fig. 10.1 with $B_1 = -5\,T$, $B_2 = 5\,T$, and $m = 0, 1$ with $n = 1$ the $-+$ stands for bonding and anti-bonding respectively. (b) Angular current versus $r$ for the eigenstates marked by open, red dots in panel (a). The lower (upper) inset to panel (b) shows the group velocity for bonding (anti-bonding) states.

\[
\zeta_\phi = \begin{pmatrix} e^{-i\phi} & 0 \\ 0 & e^{i\phi} \end{pmatrix}.
\]

(10.18)

For the special case $B_2 = -B_1 = B$ we show two split levels, for $m = 0$ and 1 in Fig. 10.4(a) and the angular current $J_\theta$ in Fig. 10.4(b) at ($r = 40$: $J_\theta$ is negative (positive) for bonding (anti-bonding) states. The insets in Fig. 10.4(b) also show the corresponding electron trajectories. As is clear from Fig. 10.3(a) for $R$ small the electron is mainly with magnetic field outside the dot with an energy corresponding to a LL outside the dot. When $R$ increases the bonding state will decrease in energy because of the smaller average magnetic field. The electron state is partially inside and outside the dot. Only when $R$ is large enough will the electron be localized inside the dot. We show the total wave function corresponding to the states indicated in Fig. 10.3(a) by open dots for $m = -1, 0, 1$ in Fig. 10.3(b).
For these values of $m$ the electron is localized around the boundary at $r = R$.

Figure 10.5: (a) Energy spectrum for the magnetic field profile shown in Fig. 10.1 with $B_1 = 2.5T$, $B_2 = 5T$, and $-1 \leq m \leq 1$. (b) Shows the wave function for the eigenstates marked by a dot in panel (a). The inset shows the classical trajectory inside and outside the dot rotating in the same direction.

In Fig. 10.5(a) we plot the energy states as a function of the radius for a dot with positive magnetic fields inside and outside the dot. In this case the classical trajectory inside and outside the dot rotate in the same direction (see inset of Fig. 10.5(b)); consequently, there are no anti-bonding states but only bonding states. The total wave function for three different states is plotted in Fig. 10.5(b).

In Fig. 10.6 the energy states are plotted as a function of the quantum number $m$ and for $B_1 = -B_2$. As shown in Fig. 10.6(a), all levels split into bonding and anti-bonding states.

In the presence of a constant 2D potential $V(x, y) = V \Theta(R - r)$ one adds this term in Eq. (10.2). The wave functions remain the same in all regions of interest but the eigenvalues do not. Accordingly, the degeneracies shown in Figs. 10.3(a) and 10.4(a) should be lifted. Indeed, this is the case as we show in Fig. 10.7 where we plot the spectrum as a function of the dot radius for antiparallel fields in (a).
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Figure 10.6: (a) Dependence of the energy spectrum on the quantum number $m$ in a magnetic dot for (a) $B_1 = -5 \text{T}$ and $B_2 = 5 \text{T}$ and (b) $B_1 = 2.5 \text{T}$ and $B_2 = 5 \text{T}$.

($B_1 = -5T$ and $B_2 = 5 T$), and parallel fields in (b) ($B_1 = 2.5T$, $B_2 = 5 T$) in the presence of the constant potentials $V_1 = 20 \text{ meV}$ inside the dot and $V_2 = 0$ outside the dot. The shown curves correspond to $m = 0, \pm 1, \pm 2$.

We now investigate whether a Dirac electron can have a zero energy state inside the dot. To find such a state we set $E = 0$ in Eqs. 10.4(a) and 10.4(b). Then the general solutions are

\[
a(r) \sim r^{m+s_1} e^{\gamma_1 r^2/2},
\]

and

\[
b(r) \sim r^{-m-1-s_1} e^{-\gamma_2 r^2/2}.
\]

In order to have a finite wave function we have to satisfy the boundary conditions. First, at $r = 0$ the wave function should behave as $r^\alpha$ ($\alpha \geq 0$) and for $r \to \infty$ the function should decay like $r^{-\alpha}$ ($\alpha \geq 1$). These conditions for component $a$ entail $m \geq -s_1$ if $r \to 0$ and $\gamma_2 < 0$ if $r \to \infty$. For the component $b(r)$, these conditions lead to $m \leq -s_1 - 1$ for $r \to 0$ and to $\gamma_2 > 0$ for $r \to \infty$.

For a magnetic dot in a homogeneous background magnetic field the magnetic field inside and outside the dot is different. For example, for $\gamma_1 < 0$ and $\gamma_2 > 0$ we have $s_1 = 0$ and $s_2 = \gamma_1 - \gamma_2$. In order to satisfy these conditions, $a(r)$ should be zero, otherwise a divergence occurs at $r \to \infty$.

For the second component $b$ the condition reads, $m \leq -1$. Then the number of degenerate zero-energy state is of the order $\approx L^2$ ($L$ is the size of the sample). The number of zero-energy states relates to the total magnetic flux which here diverges because the area of the magnetic dot as compared to the size of the sample area is too small (i.e. $L \gg R$) and the magnetic flux is proportional to $\approx L^2$. 

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Figure 10.7: (a) Energy spectrum for the magnetic field profile shown in Fig. 10.1 with \( B_1 = -5T, B_2 = 5T, \) and \(-2 \leq m \leq 2,\) in the presence of a potential step \( V_1 = 20 \text{ meV} \) and \( V_2 = 0.\) (b) The same as in (a) with \( B_1 = 2.5T.\)

10.3.2 Magnetic ring

Now we investigate possible bound states in the magnetic ring shown in Fig. 10.8. With \( r_1 = 1 - w/2 \) and \( r_2 = 1 + w/2\) the vector potential for this system is

\[
A(r) = \begin{cases} 
\frac{\gamma_1 r}{r}, & 0 < r < r_1, \\
\frac{\gamma_2 r + (\gamma_1 - \gamma_2) r^2_1}{r^2_1}, & r_1 < r < r_2, \\
\frac{\gamma_3 r + (\gamma_2 - \gamma_3) r^2_2 + (\gamma_1 - \gamma_2) r^2_1}{r}, & r > r_2. 
\end{cases} \tag{10.21}
\]
The solutions for $b(r)$ in the three different regions are

$$b(r) = \begin{cases} 
A_1 P_1 e^{-|\gamma_1| r^2/2} M (\alpha_1, \beta_1, z_1), & 0 < r < r_1, \\
A_2 P_2 e^{-|\gamma_2| r^2/2} \left[CM (\alpha_2, \beta_2, z_2) + DU (\alpha_2, \beta_2, z_2)\right], & r_1 < r < r_2, \\
B_p P_3 e^{-|\gamma_3| r^2/2} U (\alpha_3, \beta_3, z_3), & r > r_2.
\end{cases}$$  \hspace{1cm} (10.22)$$

with $\alpha_i, \beta_i,$ and $z_i$ given after Eq. (10.6).

The component $a(r)$ is obtained from Eq. 4(a). We have to satisfy the boundary conditions at $r_1 = R - W/2$ and $r_2 = R + W/2$. In Fig. 10.9(a) we plot the bound states obtained for a ring with $B_1$ antiparallel to $B_0$ and $B_2$ and all of them equal to 3 T. The width of the ring ($W = 20$ nm) is fixed and we plot the bound states as a function of $R$. With increasing $R$ all bound states approach the LL energies for a homogenous field of $B = 3$ T. In Fig. 10.9(b) and (c) we plot the total wave functions for the states marked by a circle or a square in the inset of Fig. 10.9(a), respectively. Note that the wave functions are mainly localized inside the ring region $r < R - w/2$ and partially in the ring region $R - w/2 < r < R + w/2$.

We can also obtain the expectation value of the orbital momentum $L_z$ using

$$\langle L_z \rangle = \left\langle -i\hbar \frac{\partial}{\partial \varphi} \right\rangle = \hbar \int b^* b.$$

The expectation value of $L_z$ is plotted in Fig. 10.10. As shown, with increasing $R$, $\langle L_z \rangle$ tends to $m\hbar$ while for intermediate $R$-values $\langle L_z \rangle > m\hbar$ and the difference
Figure 10.9: (a) Energy spectrum as a function of \( R \) for the ring shown in Fig. 10.8 with \( B_0 = B_2 = 3 \) T, \( B_1 = -3 \) T for \( m = 0, \pm 1 \), and \( W = 20 \) nm. (b) Wave function for the eigenstates marked by a dots or squares in the inset of panel (a) can be very large for small \( R \)-values. Please note that although our problem is circular symmetric, \( L_z \) is not conserved quantity in graphene and \( m \) is the quantum number corresponding to the operator \( J_z \) given by the sum of orbital angular momentum \( L_z \) and a term describing the pseudospin \( S_z \),

\[
J_z = L_z + S_z,
\]

where \( S_z = \hbar \sigma_z / 2 \). Using Eqs. (10.24) and (10.23) we obtain \( \langle J_z \rangle = (m + 1/2)\hbar \).

In Fig. 10.11(a) we plot the bound states as a function of the magnetic field \( (B) \) for a ring with \( B_1 = 0 \) and \( B_0 = B_2 = B \) an external magnetic field \( B_{ext} \). Notice that in Fig. 10.11(a) we have for fixed \( m \)-value several anti-crossings between...
10.4. MAGNETIC FIELD PROFILES OF FINITE EXTENT

Figure 10.10: Expectation value of the angular momentum $L_z/\hbar$ as function of $R$ for the ring shown in Fig. 10.8 with $B_0 = B_2 = 3$ T, $B_1 = -3$ T, $-1 \leq m \leq 1$, and $W = 20$ nm.

levels with different $n$-value. These anti-crossings are consequence of two different tendencies, on the area which view the $B = 0$ ring area as a small perturbation and have energy just below those of LLs in a homogenous $B$-field and states that are predominantly localized in the $B = 0$ ring area whose quantum confinement increase with $B$ but for very large $B$ its value tends to the one obtained for hard wall confinement [122,123]. When two of such states reach the same energy value they anti-cross.

The situation in Fig. 10.11(b) is very different where we have a spectrum that is not invariant under $B_{ext} \rightarrow -B_{ext}$. For $|B_{ext}| \gg B_0$ we recover the LLs for a homogenous field equal to $B_{ext}$. For intermediate values of $B_{ext}$ the degeneracy of the levels is lifted which is most pronounced for $B_{ext} \approx -B_0$. For $B_{ext}$-values the bound states are closely related to the classical-type of snake orbit.

10.4 Magnetic field profiles of finite extent

We now look for possible long-living, quasi-stationary states in graphene for magnetic field profiles shown in Fig. 10.12. Such profiles can be created by a perpendicularly magnetized ferromagnetic disk placed above a 2DEG [54] assuming that this is possible with graphene as well. To account for quasi-bound states one normally solves the time-dependent Schrödinger equation which is a very complicated problem when compared to the standard eigenvalue problem. Here we
CHAPTER 10. GRAPHENE IN INHOMOGENEOUS MAGNETIC FIELDS: BOUND, QUASI-BOUND AND SCATTERING STATES

Figure 10.11: (a) Energy spectrum as a function of the magnetic field $B$ for the ring shown in the inset. (b) Energy spectrum for a magnetic ring as a function of an external magnetic field with $B_0 = 5$ T. In both cases $R = 60$ nm and $W = 20$ nm.

Figure 10.12: (a) A magnetic dot of radius $R_1$ in a field $B_1$ surrounded by an annulus of radius $R_2$ in a field $B_2$. (b) A magnetic ring profile.
10.4. MAGNETIC FIELD PROFILES OF FINITE EXTENT

follow the method presented in detail in Ref. [118, 120], and calculate the local density of states. The idea is to confine the electron in a large region of finite radius $R_\infty \gg r_2$, with its wave function vanishing at the border ($r = R_\infty$), and treat the problem as a stationary one. The justification is that the result of a measurement, e.g., a tunneling current directed perpendicular to the dot via a STM tip or the power absorption in near-field infrared spectroscopy, depends on the average value of the electron wave function in the dot. Therefore, we introduce the integral

$$I = 2\pi \int_0^\infty r F(r) |\Psi(r)|^2 dr,$$

(10.25)

which depends on the electron probability density and is also proportional to the local density of states. The aperture function $F(r)$ characterizes the interaction of the electron with the measuring probe.

The integral in Eq. (10.25) is sensitive to the probability of finding an electron in the dot and for a quasi-bound state it will exhibit a peak corresponding to the energy of this state. The width of the peak is related to the inverse of the lifetime of this quasi-stationary state. For definiteness we use a Gaussian aperture function

$$F(r) = b R_2^2 e^{-br^2}, \quad b = R_2^{-2} \ln 10.$$

(10.26)

10.4.1 Magnetic dot

We consider a magnetic dot in a perpendicular magnetic field $B_1$ surrounded by a field $B_2$ in a finite region outside it as shown in Fig. 10.12. Explicitly the field $B(r)$ is given by

$$B(r) = \begin{cases} B_1, & 0 < r < R_1; \\ B_2, & R_1 < r < R_2, \\ 0, & R_2 < r < \infty, \end{cases}$$

(10.27)

and the corresponding vector potential by

$$A(r) = \frac{1}{r} \begin{cases} \gamma_1 r^2, & 0 < r < R_1; \\ \gamma_2 r^2 + (\gamma_1 - \gamma_2) R_1^2, & R_1 < r < R_2; \\ \gamma_2 R_2^2 + (\gamma_1 - \gamma_2) R_1^2, & R_2 < r < \infty. \end{cases}$$

(10.28)

We proceed as in Sec. 6.2 and obtain Eq. (10.4) which we convert into two second-order differential equations for the components $a(r)$ and $b(r)$. The one for $b(r)$ is again given by Eq. (10.5). Explicitly, the solutions for $b(r)$ in the three different regions are, respectively,

$$b_1(r) = A r^{m+1} e^{\gamma_1 r^2/2} M(\alpha_1, \beta_1, z_1),$$

(10.29)
Figure 10.13: (a) Local density of states $\rho(E)$ versus energy for $m = 0, \pm 1$ and $B_2 = -B_1 = 5$ T, $R_1 = 20$ nm and $R_2 = 50$ nm. The wave functions corresponding to the states marked by circles (squares) in (a) are shown in (b) and (c).

$$b_2(r) = r^{[m+1]}e^{[\gamma_2]r^2/2}$$
$$\times \{BM(\alpha_2, \beta_2, z_2) + CU(\alpha_2, \beta_2, z_2)\},$$

(10.30)

and

$$b_3(r) = GJ_\nu(|E|r) + HY_\nu(|E|r),$$

(10.31)

with $\nu = s_3 + m + 1$. $J_\nu(z)$ and $Y_\nu(z)$ are the Bessel and modified Bessel functions, respectively. The solutions for $a(r)$ are obtained from Eq. (10.4). The components $a(r)$ and $b(r)$ obey the following boundary conditions at $r = R_1$ and $r = R_2$: $a_1(R_1) = a_2(R_1)$, $b_1(R_1) = b_2(R_1)$, $a_2(R_2) = a_3(R_2)$, $b_2(R_3) = b_3(R_2)$, and $G^2 + H^2 = 1$. The last condition comes from the vanishing of the wave function for $r = R^\infty$.

In Fig. 10.13 we plot the local density of states for a finite dot with antiparallel magnetic fields inside and outside the dot for two different dot sizes. Now the energy states are broadened, i.e., they have a finite lifetime and no bound state exist. The sharp peaks for $m = 0$ and $m = 1$ in panel (a) are reminiscent for the
10.4. MAGNETIC FIELD PROFILES OF FINITE EXTENT

Figure 10.14: Quasi-bound states with orbital momentum \( m = 0 \) for \( B_1 = -5 \) T (see Fig. 10.12(b)), and \( B_2 = 5 \) T as a function of \( R_2/R_1 \) with \( R_1 = 20 \) nm fixed. The green shaded area is a measure of the inverse lifetime of these states.

previous bonding and anti-bonding states of the \( n = 1 \) split level. We also plot the total wave function for three different energies indicated by squares and circles, respectively in Figs. 10.13(b) and (c). We see that when the energy is close to the values of a quasi-bound state the probability of finding the electron inside the dot becomes large. Such states are also called resonant states. The energy of these quasi-bound states for angular momentum \( m = 0 \), i. e. for s-wave scattering, are shown in Fig. 10.14 and, as expected, for \( R_2 \gg R_1 \) the quasi-bound states will be close to the energy of the LLs (given by the dashed lines in Fig. 10.14). The width of the resonances (see Fig. 10.13(a)) are shown by shaded area in Fig. 10.14 which are proportional to the inverse life-time of these quasi-bound states.

We also show the numerical results for a magnetic dot, with parallel magnetic fields inside and outside it, in Figs. 10.15 and 10.16. Notice that qualitatively the results are rather similar except that in Fig. 10.14 the lowest energy bound state is below the LL result for \( R_2/R_1 < 2 \).

10.4.2 Magnetic ring

Next we consider a magnetic ring as shown in Fig. 10.12(b), which can be obtained from the previous magnetic field configuration by setting \( B_1 = 0 \). The new magnetic profile is \( B(r) = B\Theta([R_2 - r](r - R_1)) \) and the corresponding vector potential profile is given by

\[
A(r) = \begin{cases} 
R_1^2, & 0 < r < R_1; \\
R_2^2, & R_1 < r < R_2, \\
\gamma \frac{r}{r}, & R_2 < r < \infty.
\end{cases}
\]  

(10.32)
Figure 10.15: (a) Local density of states $\rho(E)$ versus energy for $m = -1, 0, 1$, $B_1 = 2.5$ T, and $B_2 = 5$ T, $R_1 = 20$ nm and $R_2 = 50$ nm. The wave functions corresponding to the states marked by circles (squares) in (a) are shown in (b) and (c).

The solutions for $b(r)$ in the three different regions are, respectively,

$$b_1(r) = AJ_{\nu_1}(|E|r),$$  \hspace{1cm} (10.33)

with $\nu_1 = s_1 + m + 1$ and $s_1 = \gamma R_1^2$.

$$b_2(r) = r^{[m+1]}e^{\gamma|z|^2/2}\left\{BM(\alpha, \beta, z) + CU(\alpha, \beta, z)\right\},$$  \hspace{1cm} (10.34)

and

$$b_3(r) = GJ_{\nu_2}(|E|r) + HY_{\nu_2}(|E|r),$$  \hspace{1cm} (10.35)

with $\nu_2 = s_3 + m + 1$ and $s_3 = \gamma R_2^2$.

We obtained the local density of states and quasi-bound states of this system numerically. In Fig. 10.16(a) we plot the local density of states for three different quantum numbers $m$. The total wave function is plotted for two different cases.
10.5. MAGNETIC DOT WITH \( \langle B \rangle = 0 \)

When the energy is close to that of a quasi-bound state (b) the electron is localized inside the ring, cf. Fig. 10.17(b). When it is not, cf. Fig. 10.17(c), the electron does not penetrate the ring area. The results for the energy and width of the resonant states are qualitatively very similar as depicted in Fig. 10.16 and are therefore not shown.

10.5 Magnetic dot with \( \langle B \rangle = 0 \)

A magnetic dot with zero average magnetic field \( \langle B_z \rangle = 0 \) is the structure which can be realized experimentally by depositing e.g. Dy micromagnets on top of graphene with an insulating layer in-between to prevent electrical contact, as was previously realized on top of a GaAs/Al\(_x\)Ga\(_{1-x}\)As heterostructure [124,125]. We model the magnetic field profile by a simple step as depicted in Fig. 10.19. The field \( B(r) \) is

\[
B(r) = \begin{cases} 
B_1, & r < R_1 \\
B_2, & R_1 < r < R_2 \\
0, & r > R_2 
\end{cases}
\]  

(10.36)

The condition \( \langle B_z \rangle = 0 \) is satisfied for \( B_2 = -B_1/(R_2^2/R_1^2 - 1) \). The solutions in the three different regions are the same as Eqs. (10.29), (10.30) and (10.31).

Such a system can support only quasi-bound states. The numerical results for the local density of states are shown in Fig. 10.19 for two different sizes of magnetic dot and different quantum numbers \( m \). As different from previous cases we see that for \( m \geq 0 \) there are pronounced peaks close to zero energy. When the
CHAPTER 10. GRAPHENE IN INHOMOGENEOUS MAGNETIC FIELDS: BOUND, QUASI-BOUND AND SCATTERING STATES

Figure 10.17: (a) Local density of states \( \rho(E) \) versus energy for \( m = -1, 0, 1 \) for the magnetic ring profile shown in Fig. 10.12(b) with \( B = 5 \) T, \( R_1 = 20 \) nm and \( R_2 = 50 \) nm. The wave functions corresponding to the symbols in (a) are shown in (b) and (c).

ratio \( R_2/R_1 \) increases we found that these peaks become sharper indicating long-living quasi-bound states. Later on we will shown that these states give rise to a pronounced structure in the magnetoresistance and the Hall resistance. The corresponding wavefunctions are shown in Fig. 10.19(c) and those at the energy of the first LL in Fig. 10.19(b).

10.5.1 Zero energy state for a finite magnetic dot

The solution presented in Sec. 6.3 should be modified in the case of a finite magnetic dot. Here we have three regions and the solution in the third region (i.e.
10.5. MAGNETIC DOT WITH $\langle B \rangle = 0$

outside the magnetic dot profile where $B = 0$ is

$$a(r) \sim r^{m+s_3}$$  \hspace{1cm} (10.37)

and

$$b(r) \sim r^{-m-1-s_3}.$$  \hspace{1cm} (10.38)

In order to have a zero-energy state we should have $m \leq -s_3$ for the component $a(r)$ and $m \geq -s_3$ for the component $b(r)$. From the fact that $a(r)$ is converging in the first region for $m \geq -s_1$ and $b(r)$ for $m \leq -s_1 - 1$, the zero-energy states for the previously discussed structures, are as follows.

1) Magnetic dot of finite size (cf. Fig. 10.12(a)). In this case $s_1 = 0$ and $s_3 = \gamma_2 R_2^2 + (\gamma_1 - \gamma_2) R_1^2 = \Phi/\phi_0$, where $\Phi$ is the total magnetic flux with $\phi_0 = \hbar/e$. Then $a(r)$ and $b(r)$ should satisfy the conditions

$$ \begin{cases} 
  a(r) \to 0 & \leq m < -[\Phi/\phi_0] \\
  b(r) \to -[\Phi/\phi_0] - 1 & < m \leq -1 
\end{cases} $$  \hspace{1cm} (10.39)

where $[\Phi/\phi_0] = n$ is the largest integer smaller than $\Phi/\phi_0$. These two conditions cannot be satisfied at the same time. Then $a(r) = 0$ for $\Phi > 0$ and the second condition is true. In order to have zero-energy state solutions we have to limit the angular momentum $m$ for the second component as $-2 \leq m \leq -[\Phi/\phi_0] - 1$ which leads to $0 \leq m \leq -1$.

2) Magnetic ring of finite size (cf. Fig. 10.12(b)). In this case we have ring $s_1 = \gamma_1 R_1^2 = \Phi_1/\phi_0$ and $s_3 = \gamma_2 R_2^2 = \Phi_2/\phi_0$. Repeating the procedure above we find that zero-energy states exist under the condition $-2 \leq m \leq -[\Phi_2/\phi_0] - 1 = -(1 + \Phi_1/\phi_0)$.

3) Magnetic dot with $\langle B_z \rangle = 0$ (cf. Fig. 10.19). Because the average magnetic field is zero, the total flux is zero and we do not have any zero-energy states. It is also possible to show that a zero energy solution for a finite-size magnetic dot is not acceptable here because $s_3 = 0$, $[\Phi/\phi_0] = 0$ which leads to $0 \leq m \leq -1$ that can not be satisfied.

10.5.2 Elastic scattering

Next we concentrate on scattering problem of Dirac electrons by a circular symmetric magnetic dot with $\langle B \rangle = 0$. The layout of the problem is shown in Fig. 10.19. We assume that electrons are coming from $-\infty$, along the $x$ axis, and calculate the probability for them to be scattered and deflected by an angle $\varphi$. The wave function of a free electron propagating along the $x$ axis (towards $+\infty$) is

$$\Psi_0(r) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{ikx}$$  \hspace{1cm} (10.40)
with $k > 0$. It describes a homogeneous electron flow with density $\rho = 1$, and current $J = \{1, 0\}$.

In standard scattering theory the wave function far away from the scatterer is presented as a sum of two parts,

$$\Psi(r) \approx \Psi_0(r) + \frac{f(\varphi)}{\sqrt{r}} e^{ikr};$$  \hspace{1cm} (10.41)

the first part corresponds to the incoming electron while the second part, called scattering amplitude, is composed of two components (as the wave function itself):

$$f = \left( \begin{array}{c} f_1 \\ f_2 \end{array} \right).$$  \hspace{1cm} (10.42)

The macroscopic scattering characteristic is the differential cross-section which is defined as the number of electrons falling into the angle element $d\varphi$ per unit time, namely, the electron velocity multiplied by the length $rd\varphi$ of a rather large-radius circle, where this electron flow is measured. Having in mind the definition $J = \Psi^+ \sigma \Psi$ we define the differential cross-section as follows:

$$d\sigma(\varphi) = P(\varphi)d\varphi = f^+(\varphi)(\sigma \cdot n)f(\varphi)d\varphi.$$  \hspace{1cm} (10.43)

Here $n$ stands for the unit vector perpendicular to the above mentioned circle and
Figure 10.19: (a) Local Density of states for $m = 0, \pm 1, \pm 2, \pm 3$ for the magnetic field profile shown in Fig. 10.19 with $B_1 = -5T$ and $(R_1, R_2) = (30, 80)$ nm. The dashed lines shows the position of the LLs. (b) Total wave function for the first LL indicated by a circle for different values of $m$. (c) As in (b) for the peaks indicated by squares in (a).

$P(\varphi)$ is given by

$$P(\varphi) = e^{i\varphi}a^*b + e^{-i\varphi}a^*b.$$  \hspace{1cm} (10.44)

The total cross-section is then given by

$$\sigma = \int_0^{2\pi} P(\varphi)d\varphi.$$  \hspace{1cm} (10.45)

We express the solution outside the dot as a combination of Bessel functions

$$a(r) = w_n \left\{ \cos \delta_m \cdot J_m(kr) + \sin \delta_m \cdot Y_m(kr) \right\}.$$  \hspace{1cm} (10.46)
CHAPTER 10. GRAPHENE IN INHOMOGENEOUS MAGNETIC FIELDS: BOUND, QUASI-BOUND AND SCATTERING STATES

Then the components of the eigenfunction are related by

\[ b(r) = \frac{1}{E} \left\{ \frac{d}{dr} - \frac{m}{r} \right\} a(r) = w_n \left\{ \cos \delta_m \cdot J_{m+1}(kr) + \sin \delta_m \cdot Y_{m+1}(kr) \right\}. \]  \(10.47\)

This leads to the following expansion:

\[ \psi_1(r, \varphi) = \sum_{m=-\infty}^{\infty} e^{im\varphi} w_n \times \left\{ \cos \delta_m \cdot J_m(kr) + \sin \delta_m \cdot Y_m(kr) \right\}, \]  \(10.48\)

\[ \psi_2(r, \varphi) = i \sum_{m=-\infty}^{\infty} e^{i(m+1)\varphi} w_n \times \left\{ \cos \delta_m \cdot J_{m+1}(kr) + \sin \delta_m \cdot Y_{m+1}(kr) \right\}. \]  \(10.49\)

for the components of the wave function. The coefficients \(w_n\) and \(\delta_m\) are determined by the boundary conditions on \(r_1, r_2\) and the wave function (10.40).

In the asymptotic region \((r \to \infty)\) we have the following asymptotes for the Bessel functions: \(J_m(kr) = (c/\sqrt{r}) \cos \Delta_m\) and \(Y_m(kr) = (c/\sqrt{r}) \sin \Delta_m\), with \(\Delta_m = kr - \frac{\pi}{2} m - \frac{\pi}{4}\), where \(c = \sqrt{2/\pi k}\). They enable us to present Eqs. (10.48) and (10.49) in the asymptotic region as

\[ \psi_1(r) = \frac{c}{\sqrt{r}} \sum_{m=-\infty}^{\infty} w_m e^{im\varphi} \cos(\Delta_m - \delta_m), \]  \(10.50\)

Figure 10.20: The phase shift \(\delta_m\) for \(m = 0, \pm 1, \pm 2, \pm 3\) as a function of the energy for \(B_1 = -5T\), for \((R_1, R_2) = (30, 80)\) nm.
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$$\psi_2(r) = \frac{c}{\sqrt{r}} \sum_{m=-\infty}^{\infty} w_m e^{i(m+1)\phi} \cos(\Delta_{m+1} - \delta_m). \quad (10.51)$$

These expansions must agree with the asymptotic (10.40). For this purpose we write the exponential in Eq. (10.40) as

$$e^{ikr} = e^{ikr \cos \phi} = \sum_{m=-\infty}^{\infty} i^m e^{im\phi} J_m(kr)$$

$$\approx \frac{c}{\sqrt{r}} \sum_{m=-\infty}^{\infty} i^m e^{im\phi} \cos \Delta_m \quad (10.52)$$

$$= \frac{c}{\sqrt{r}} \sum_{m=-\infty}^{\infty} i^m e^{im\phi} (e^{i\Delta_m} + e^{-i\Delta_m}).$$

Figure 10.21: Total cross section for $B_1 = -5T$, (a) $(R_1, R_2) = (30, 80)$ nm and (b) $(R_1, R_2) = (50, 80)$ nm.

First, we compare Eq. (10.50) with the first wave function component (10.48). Rewriting the asymptotic of this component as

$$\psi_1(r) = \frac{c}{\sqrt{r}} \sum_{m=-\infty}^{\infty} w_m e^{im\phi} \left\{ e^{i(\Delta_m - \delta_m)} + e^{-i(\Delta_m - \delta_m)} \right\}. \quad (10.53)$$

The coefficients of the exponents representing the incoming wave (the second term inside the curly brackets) must be equal. This gives

$$w_m = i^m e^{-i\delta_m}. \quad (10.54)$$
Subtracting the asymptotic from Eq. (10.53) gives the first component of the scattered wave function part

$$
\psi^{(\text{scatt})}_1(r) = \frac{c}{\sqrt{r}} \sum_{m=-\infty}^{\infty} i^m e^{im\varphi} e^{i\Delta_m} \left\{ e^{-2i\delta_m} - 1 \right\}. \tag{10.55}
$$

Now we have to check whether the second wave function component is correct in the asymptotic region. The second sum representing the incoming wave has to be the same as in the first component. This second component can be written as

$$
\psi_2(r) = \frac{c}{\sqrt{r}} \sum_{m=-\infty}^{\infty} i^{m+1} e^{-i\delta_m} e^{i(m+1)\varphi} \times \left\{ e^{i(\Delta_{m+1}+\delta_m)} + e^{-i(\Delta_{m+1}+\delta_m)} \right\}. \tag{10.56}
$$

We can rewrite the scattered part of wave function components in the following final form:

$$
\psi^{(\text{scatt})}_1(r) = \frac{c}{\sqrt{r}} \sum_{m=-\infty}^{\infty} i^m e^{im\varphi} e^{i\Delta_m} \left\{ e^{-2i\delta_m} - 1 \right\}, \tag{10.57}
$$

$$
\psi^{(\text{scatt})}_2(r) = \frac{c}{\sqrt{r}} \sum_{m=-\infty}^{\infty} i^m e^{im\varphi} e^{i\Delta_m} \left\{ e^{-2i\delta_{m-1}} - 1 \right\}. \tag{10.58}
$$
10.5. MAGNETIC DOT WITH $\langle B \rangle = 0$

This enables to write the components of the scattering amplitude (10.42) in the form

$$f_1 = e^{-i\pi/4} \frac{c}{\sqrt{T}} \sum_{m=-\infty}^{\infty} e^{im\varphi} \left\{ e^{-2i\delta_m} - 1 \right\},$$  \hspace{1cm} (10.59a)

$$f_2 = e^{-i\pi/4} \frac{c}{\sqrt{T}} \sum_{m=-\infty}^{\infty} e^{im\varphi} \left\{ e^{-2i\delta_{m-1}} - 1 \right\},$$  \hspace{1cm} (10.59b)

the differential cross-section (10.44) as

$$P(\varphi) = \frac{4}{\pi k} \sum_{m,m'} e^{i[(m-m')\varphi-(\delta_m-\delta_{m'})]} \sin \delta_m \sin \delta_{m'},$$  \hspace{1cm} (10.60)

and the total cross-section as

$$\sigma(E) = \frac{8}{k} \sum_{m=-\infty}^{\infty} \sin^2 \delta_m(E).$$  \hspace{1cm} (10.61)

For a random distribution of dilute non-overlapping scatters, the zero temperature magnetoresistance and Hall resistance are given by [126]

$$\rho_{xx}/\rho_0 = \int_{-\pi}^{\pi} d\varphi w(k,f) (1 - \cos \varphi)$$

$$= \sum_{m=-\infty}^{\infty} 4 \sin^2 (\delta_m - \delta_{m+1})$$

$$\rho_{xy}/\rho_0 = \int_{-\pi}^{\pi} d\varphi w(k,f) \sin \varphi$$

$$= \sum_{m=-\infty}^{\infty} 2 \sin [2(\delta_m - \delta_{m+1})]$$

with $\rho_0 = (1/4\pi^2)(n_0/n_e)(\hbar/e^2)$ where $n_e$ is the electron concentration, $n_0$ the concentration of magnetic scatterers, and $w(k,f) = kP(\varphi)$ is the probability for an electron with wave vector $k$ to be scattered by an angle $\varphi$.

In Fig. 10.19 we showed the local density of states as a function of energy for $(R_1, R_2) = (30, 80)$ with $B_1 = 5$ T. The resonances are near the position of the LLs as shown by the vertical dashed lines. For $R_1$ small we have some quasi-bound states between the $E = 0$ and the first LLs for $m > 0$. These levels moves close to the $E = 0$ one if we increase $R_1$. The peaks shifts $\delta_m$ are shown in in Fig. 10.20 where resonances are visible for certain energy values with jumps in $\delta_m$. 

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In Fig. 10.21(a) and (b) we plot the total cross section as a function of $E$. Classically and in 2D this is equal to the total diameter of the magnetic inhomogeneity $\sigma = 2R_b$. The resonances shown up as small peaks, correspond to the quasibound states of Fig. 10.19(a). Notice that the peaks in Fig. 10.21(a) for small energies ($E < 50$) are absent in Fig. 10.21(b). The difference comes from the fact that when we increase the $R_1$ the structure behaves more or less like a finite magnetic dot. As discussed in Sec. V. A zero-energy states exist for $0 \leq m < -\Phi/\phi_0$. Here all bound states in the finite size magnetic dot become quasi-bound states because of the zero total magnetic flux. For $R_1$ large these levels are close to the $E = 0$ level whereas for $R_1$ small these quasi-bound states move away from the $E = 0$ level.

The corresponding magnetoresistance and Hall resistance are shown in Fig. 10.22(a) and(b) for the same dot structures. We found different behavior in two energy regimes: 1) For $0 < E < E_1$ (here $E_1$ is the first LL $E \approx 81$ meV) all resonances result from the quasi-bound states shown in Fig. 10.19(a). These resonances are not found in the normal 2DEG and are unique for graphene. 2) For $E > E_1$ there are two types of resonances: first those which occur at the energy of the LLs of the inner core of the magnetic-field profile and second those corresponding to quasi-bound snake orbit states that are located near the interface between the $B > 0$ and $B < 0$ regions.

10.6 conclusions

In this chapter we studied the bound, quasi-bound and scattered states for electrons in graphene in the presence of circular inhomogeneous magnetic field profiles. The corresponding spectra were investigated as a function of the size and radii, the strength of the inhomogeneous magnetic field and of a uniform background field, and the angular momentum quantum number.

We considered the eigenvalue problem of a model quantum magnetic dot in the presence of a background field where the homogeneous magnetic field perpendicular to the 2D electron motion plane is created only in a finite region in a circle of radius $R$. We studied the bound states for two different cases: 1) when inner and outer magnetic field have different sign ($B_1 < 0$ and $B_2 > 0$). In this case we found that the energy levels are split into bonding and anti-bonding states, and 2) when both inner and outer magnetic field have same sign.

We also studied the bound states in the case of a magnetic ring in the presence of an external magnetic field.

Magnetic dot profiles of finite extent behave very differently. In this case the magnetic field fails to confine electrons. Although in such a magnetic field profile
no confined states are found, quasi-bound sates with a finite lifetime are present. We presented a study of the local density of states and its dependence on the dot radius. The broadening of the peaks in the LDOS (i.e. the inverse lifetime of the quasi-bound state) is mainly caused by the touching of electron wave function tail with the magnetic dot edge.

Special attention was paid to the zero energy states for all different magnetic dots and we showed that a zero energy bound state exists when the magnetic flux is non-zero.

Finally a magnetic dot with $\langle B_z \rangle = 0$ was considered. We calculated the local density of states, the elastic scattering, the magnetoresistance and the Hall resistance. All the zero energy states that existed in the case of finite magnetic dots become quasi-bound states. These quasi-bound states are located close to $E = 0$ and are found only in the case of Dirac electron. This results into two different energy regions in the magnetoresistance and the Hall resistance. They differ by the presence of sharp peaks due to resonant scattering as a result of the existing of quasi-bound states.
Scattering of Dirac electrons by circular mass barriers: valley filter and resonant scattering

Abstract. In this chapter the scattering of two-dimensional (2D) massless Dirac electrons is investigated in the presence of a random array of identical circular mass barriers. The inverse momentum relaxation time and the Hall factor are calculated and used to obtain parallel and perpendicular resistivity components within linear transport theory. We found a non zero perpendicular resistivity component which has the opposite sign for electrons in the different $K$ and $K'$ valleys. This property can be used for valley filter purposes. The total cross-section for scattering on penetrable barriers exhibit resonances due to the presence of quasi-bound states in the barriers that show up as sharp gaps in the cross-section while for Schrödinger electrons they appear as peaks.

11.1 Introduction

During the last decades there has been a lot of theoretical and experimental attempts to use the spin of the electron as a carrier of information [127]. Graphene in addition to the spin of the electron has two more degrees of freedom, sublattice pseudospin and valley isospin or valley index. In order to scatter an electron from the $K$ valley to the $K'$ valley a large transfer of momentum is needed. Typical disorder and Coulomb-type of scattering is unable to provide this momentum and in such a case the valley isospin is a conserved quantum number in electronic transport. This allows us to use valley isospin as a carrier of information. It was shown that graphene nanoribbons with zigzag edges [128, 129] can be used as a valley filter. Another promising possibility to control the valley index of electrons is by using line defects [130]. These can be formed in graphene when grown on a

Nickel substrate or by using so called mass barriers that can be created by proper arrangement of dopants in the graphene sheet [131, 132]. Another way to control valley polarization is by using local strain in graphene which induces an effective inhomogeneous magnetic field with opposite sign in $K$ and $K'$ valleys, see Refs. [34, 68, 133–135].

The purpose of this chapter is to apply the above mentioned ideas to electron transport in the presence of circular mass barriers. We solve the Dirac electron scattering problem on a sharp circular mass barrier and calculated the cross-section, the inverse momentum relaxation time and the probability for the electron to be reflected in the perpendicular direction. In spite of the circular symmetry of the scatterers we obtain a non zero perpendicular component of resistivity that allows us to separate electrons with different chirality, or belonging to $K$ and $K'$ valleys.

The scattering of Dirac electrons by a penetrable circular mass barrier is influenced by the presence of quasi-bound states that results in resonant behavior. The obtained results are compared with those for standard Schrödinger electrons.

### 11.2 Problem

We consider a Dirac electron interacting with circular barrier structures shown in Fig. 11.1 by the shadowed regions. In the long wave approximation it is described by the stationary equation

$$\{H - E\} \Psi = 0$$

with the following Dirac Hamiltonian:

$$H_D = \begin{pmatrix} \sigma \cdot p + \kappa \sigma_z & 0 \\ 0 & \sigma' \cdot p - \kappa' \sigma_z \end{pmatrix}.$$  

This $4 \times 4$ matrix Hamiltonian describes low energy excitations in $K$ and $K'$ valleys. Due to its diagonal form it is possible to separate the scattering problems in...
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each $K$ or $K'$ valley. We choose the following $2 \times 2$ Hamiltonians:

$$H = \sigma \cdot \mathbf{p} + \kappa (\mathbf{r}) \sigma_z,$$  \hspace{1cm} (11.3a)

$$H' = \sigma^* \cdot \mathbf{p} - \kappa'(\mathbf{r}) \sigma_z,$$ \hspace{1cm} (11.3b)

where $\sigma = \{\sigma_x, \sigma_y\}$ and $\sigma_z$ stand for the Pauli matrices, and $\kappa, (\mathbf{r}), \kappa' (\mathbf{r})$ characterizes the mass barrier for $K$ and $K'$ electrons, respectively. We use dimensionless variables where velocities are measured in Fermi velocity unit $v_F$, all coordinates are measured in the radius $R$ of the circular scattering barrier, shown in Fig. 11.1 by the solid red line, and the electron energy — in $\hbar v_F / R$ units. From now on all equations are for $K$ valley electrons, except if otherwise specified.

According to standard scattering theory we present the wave function as

$$\Psi = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{iE \mathbf{x}} + f(\phi) \sqrt{r} e^{iE_r},$$ \hspace{1cm} (11.4)

consisting on the incident wave in the $x$-direction and the scattered part. The scattered part is characterized by the two component scattering amplitude

$$f(\phi) = \begin{pmatrix} A \\ B \end{pmatrix}.$$ \hspace{1cm} (11.5)

As the incoming wave function part is normalized to unit flow density the differential cross-section is equal to the radial flow of electrons corresponding to the scattered wave function part, namely,

$$\sigma(\phi) = f^+(\phi) (\sigma \cdot \mathbf{n}) f(\phi) = e^{i\phi} AB^* + e^{-i\phi} A^* B,$$ \hspace{1cm} (11.6)

where $\mathbf{n} = (\cos \phi, \sin \phi)$ is the unit vector in the considered direction.

Besides the above differential cross-section we shall consider the total cross-section

$$\sigma = \int_0^{2\pi} d\phi \sigma(\phi),$$ \hspace{1cm} (11.7)

and two more averages: the inverse electron momentum relaxation time (the quantity proportional to the dissipative component of resistivity)

$$\gamma = \int_0^{2\pi} d\phi \sigma(\phi) (1 - \cos \phi),$$ \hspace{1cm} (11.8)

and the quantity

$$\eta = \int_0^{2\pi} d\phi \sigma(\phi) \sin \phi,$$ \hspace{1cm} (11.9)
which corresponds to the perpendicular component of resistivity (or the analog of the Hall component in the case with magnetic field).

Due to the azimuthal symmetry of our problems it is convenient to use polar coordinates. Thus, assuming the total wave function as

\[ \Psi(r) = \begin{pmatrix} U(r) \\ V(r) \end{pmatrix}, \]  

(11.10)
we shall solve the set of equations

\[ e^{-i\varphi} \left( \frac{\partial}{\partial r} - \frac{i}{r} \frac{\partial}{\partial \varphi} \right) V = i(E - \kappa)U, \]  

(11.11a)
\[ e^{i\varphi} \left( \frac{\partial}{\partial r} + \frac{i}{r} \frac{\partial}{\partial \varphi} \right) U = i(E + \kappa)V \]  

(11.11b)

for the wave function components.

Now we expand the wave function into partial waves

\[ \begin{pmatrix} U(r) \\ V(r) \end{pmatrix} = \sum_{m=-\infty}^{\infty} w_m e^{im\varphi} \begin{pmatrix} u_m(r) \\ i e^{i\varphi} v_m(r) \end{pmatrix}, \]  

(11.12)

replacing Eqs. (11.11) by the following set of two radial equations:

\[ \left( \frac{d}{dr} + \frac{m+1}{r} \right) v_m = (E - \kappa)u_m, \]  

(11.13a)
\[ \left( \frac{d}{dr} - \frac{m}{r} \right) u_m = -(\kappa + E)v_m. \]  

(11.13b)

These equations are our main instrument when considering the problems shown in Fig. 11.1.

### 11.3 Boundary conditions

For the sake of simplicity we restrict ourselves to model problems with large mass potentials, and replace the potentials by proper boundary conditions on the electron wave functions. In fact, this is the standard way of describing low energy scattering. For this purpose we have to solve the appropriate equations in the barrier region, to apply the standard boundary conditions for both wave function components on the solid circles shown in Fig. 11.1, and to calculate the limit \( \kappa \to \infty \).
start with the system shown in Fig. 11.1(c). Thus, we have to solve the following approximate set of radial equations:

\[
\begin{align*}
\frac{dv}{dr} &= -\kappa u, \\
\frac{du}{dr} &= -\kappa v
\end{align*}
\] (11.14a)

in the thin shadowed region II which is delimited by two circles of radius \(1 \pm \delta\) (\(\delta \ll 1\)). Its solution reads

\[
\begin{align*}
u &= Fe^{\kappa(r-1)} + Ge^{-\kappa(r-1)}, \\
v &= -Fe^{\kappa(r-1)} + Ge^{-\kappa(r-1)}.
\end{align*}
\] (11.15a)

Now satisfying the boundary conditions on the two circles demarcating the region II we obtain the following set of four algebraic equations

\[
\begin{align*}
u I (1 - \delta) &= Fe^{-\kappa\delta} + Ge^{\kappa\delta}, \\
v I (1 - \delta) &= -Fe^{-\kappa\delta} + Ge^{\kappa\delta}, \\
u III (1 + \delta) &= Fe^{\kappa\delta} + Ge^{-\kappa\delta}, \\
v III (1 + \delta) &= -Fe^{\kappa\delta} + Ge^{-\kappa\delta}.
\end{align*}
\] (11.16a)

Eliminating the coefficients \(F\) and \(G\) we obtain in the limit \(\delta \ll 1\) the boundary conditions

\[
\begin{align*}
v III (1) - v I (1) &= -\{u III (1) + u I (1)\} \tanh(\kappa\delta), \\
u III (1) - u I (1) &= -\{v III (1) + v I (1)\} \tanh(\kappa\delta).
\end{align*}
\] (11.17a)

connecting wave function components in the regions I and III.

For a very thin and very high mass barrier (the analog of \(\delta\)-type barrier for Schrödinger electrons, see Sec. 11.8.1) we take the following limits:

\[
\delta \to 0, \quad \kappa \to \infty, \quad \tanh(\kappa\delta) = P = \text{const},
\] (11.18)

what enables us to rewrite Eqs. (11.17) as

\[
\begin{align*}
v III (1) - v I (1) &= -P \{u III (1) + u I (1)\}, \\
u III (1) - u I (1) &= -P \{v III (1) + v I (1)\}.
\end{align*}
\] (11.19a)
These boundary conditions can be formally replaced by inserting Dirac δ-functions into Eqs. (11.13), namely, replacing those equations by

\[ \left( \frac{d}{dr} + \frac{m + 1}{r} \right) v_m = [E - 2P\delta(r - 1)] u_m, \]  

\[ \left( \frac{d}{dr} - \frac{m}{r} \right) u_m = - [2P\delta(r - 1) + E] v_m, \]

if we assume the following rule for calculating the integrals when the integrand is a product of Dirac δ-function and some function \( f(x) \) with the discontinuity [136]:

\[ \lim_{\alpha \to +0} \int_{-\alpha}^{\alpha} dx \delta(x) f(x) = \frac{1}{2} \{ f(+0) + f(-0) \}. \]

The parameter \( P \) characterizes the effective strength of the δ-type barrier, and never exceeds the value \( P = 1 \) in contrast to the case of Schrödinger electrons where it can take any value. A second major difference is that the wave function components \( u(r) \) and \( v(r) \) are discontinuous at the position of the δ-function (but the probability density is continuous) while for Schrödinger electrons the wave function is continuous but the derivative of the wave function is discontinuous in that position. This is a consequence of the fact that the Dirac-Weyl equation is a first order differential equation while the Schrödinger equation is second order.

The obtained boundary conditions for the general case shown in Fig. 11.1(c) enables us to construct analogous boundary conditions for the two other cases shown by Figs. 11.1(a,b). So, in the case of Fig. 11.1(a) we assume

\[ \kappa = \infty, \quad P = 1, \quad u_{III}(1) = v_{III}(1) = 0, \]  

and rewrite the boundary conditions given by Eqs. (11.19) as

\[ u_I(1) = v_I(1). \]

This is the boundary condition for the quantum dot, surrounded by an infinite mass barrier.

In the case of Fig. 11.1(b) an analogous reasoning leads to the following boundary condition:

\[ u_I(1) = -v_I(1), \]

that we shall use for describing Dirac electron scattering by a hard wall anti-dot.

The obtained boundary conditions enables us to neglect the \( \kappa \) terms in Eqs. (11.13) and solve the Dirac equations for free electrons

\[ \left( \frac{d}{dr} + \frac{m + 1}{r} \right) v_m = Eu_m, \]  

\[ \left( \frac{d}{dr} - \frac{m}{r} \right) u_m = -Ev_m, \]
In regions $I$ and $III$ separately.

### 11.4 Bound states in the dot

The most simple problem is the one of a quantum dot shown in Fig. 11.1(a). In this case the solution of Eqs. (11.25) in region $I$ has to be finite at $r = 0$ and is given by Bessel functions

\[
\begin{align*}
    u(r) &= F J_m(E r), \\
    v(r) &= F J_{m+1}(E r).
\end{align*}
\]

(11.26a)(11.26b)

Satisfying boundary condition (11.23) we immediately arrive at the algebraic equation

\[
J_m(E) - J_{m+1}(E) = 0
\]

(11.27)

that determines the energy of the bound states.

### 11.5 Scattering by an impenetrable circle

Now we shall consider our main problems, namely, the scattering of Dirac electrons by circular mass barriers. We shall start with the case presented in Fig. 11.1(b) — the scattering by an impenetrable circle (or by a hard wall anti-dot). According to standard scattering theory we have to construct the total wave function (11.10) solving the Dirac equations for free electrons (11.25) in the outer region $I$ that satisfies the boundary condition (11.24), to exclude the incoming part of the wave function, and calculate the cross-section by means of Eq. (11.6).

So, the solution of Eqs. (11.25) in the outer region $I$ reads

\[
\begin{align*}
    u_m(r) &= w_m [J_m(E r) \cos \delta_m + Y_m(E r) \sin \delta_m], \\
    v_m(r) &= w_m [J_{m+1}(E r) \cos \delta_m + Y_{m+1}(E r) \sin \delta_m].
\end{align*}
\]

(11.28a)(11.28b)

where the symbols $J_m$ and $Y_m$ stand for Bessel and Neumann functions, respectively.

Now satisfying the boundary conditions (11.24) for any partial wave function harmonically we obtain the expansion coefficients $\sin \delta_m$ and $\cos \delta_m$ through the so called phase shifts

\[
\tan \delta_m = -\frac{J_m(E) + J_{m+1}(E)}{Y_m(E) + Y_{m+1}(E)}.
\]

(11.29)

Usually the exclusion of the incoming plane wave from the total wave function (11.12) is done in the asymptotic region where $Er \gg 1$. Here we use the
asymptotic of the Bessel functions $J_m(Er) \approx \sqrt{2/\pi Er} \sin \Delta_m$, $Y_m(Er) \approx \sqrt{2/\pi Er} \sin \Delta_m$

\begin{equation}
\Delta_m = Er - \frac{\pi}{2} m - \frac{\pi}{4},
\end{equation}

which allows us to write the total wave function components as

\begin{align*}
U(r) &= \sqrt{\frac{2}{\pi kr}} \sum_{m=-\infty}^{\infty} w_m e^{im\phi} \cos(\Delta_m - \delta_m), \\
V(r) &= i\sqrt{\frac{2}{\pi kr}} \sum_{m=-\infty}^{\infty} w_m e^{i(m+1)\phi} \cos(\Delta_{m+1} - \delta_m).
\end{align*}

In this asymptotic region the incoming plane wave can be presented as

\begin{equation}
e^{iEx} = \sum_{m=-\infty}^{\infty} i^m e^{im\varphi} J_m(Er) \approx \sqrt{\frac{2}{\pi Er}} \sum_{m=-\infty}^{\infty} i^m e^{im\varphi} \cos \Delta_m
\end{equation}

\begin{equation}
= \sqrt{\frac{1}{2\pi Er}} \sum_{m=-\infty}^{\infty} i^m e^{im\varphi} (e^{i\Delta_m} + e^{-i\Delta_m}).
\end{equation}

Now in order to compensate the incoming term in the total wave function (11.12) by the second term of the last line in Eq. (11.32) we have to take

\begin{equation}
w_m = \frac{1}{\sqrt{2}} i^m e^{-i\delta_m}.
\end{equation}

It is remarkable that this choice makes the above mentioned compensation in both scattering amplitude components $A$ and $B$, but not in every pair of radial components $u_m$ and $v_m$ separately. This is related to the fact that the angular momentum is not a conserved quantity but that the Dirac-Weyl Hamiltonian commutes with operator consisting of the angular momentum plus isospin. So, inserting the above expression of $w_m$ into Eq. (11.31) and subtracting the incoming wave function part given by Eq. (11.32) we arrive after laborious but straightforward calculations at the following expression for the components of the scattering amplitude (11.5):

\begin{align*}
A &= e^{-3i\pi/4} \sqrt{\frac{1}{\pi E}} \sum_{m=-\infty}^{\infty} e^{im\varphi} e^{-i\delta_m} \sin \delta_m, \\
B &= e^{-3i\pi/4} e^{i\varphi} \sqrt{\frac{1}{\pi E}} \sum_{m=-\infty}^{\infty} e^{im\varphi} e^{-i\delta_m} \sin \delta_m.
\end{align*}
Inserting them into Eq. (11.6) we obtain the following differential cross-section:

\[
\sigma(\varphi) = \frac{2}{\pi E} \sum_{m,m'=-\infty}^{\infty} e^{i[(m-m')\varphi-(\delta_m-\delta_{m'})]} \sin \delta_m \sin \delta_{m'}. \tag{11.35}
\]

We have to keep in mind that the derivation of this cross-section was performed with the Hamiltonian (11.3a), which is valid for electrons in the \( K \) valley.

To obtain the results for \( K' \) valley electrons we have to repeat the procedure starting with Hamiltonian (11.3b). Fortunately, it leads to the same set of differential equations (11.11) with a single change \( U \leftrightarrow V \). Further, we replace Eq. (11.12) by

\[
\left( \frac{U(r)}{V(r)} \right) = \sum_{m=-\infty}^{\infty} w_m e^{-im\varphi} \left( \frac{u_m(r)}{-ie^{-i\varphi}v_m(r)} \right), \tag{11.36}
\]

and arrive at the same radial equation set (11.13) as was obtained for the \( K \) valley case. Consequently, all equations, including the boundary condition, remain the same for the \( K' \) valley as well. The equation for the differential cross-section for the \( K' \) valley, however, differs. In this case the changes \( m \to -m \) and \( m' \to -m' \) have to be performed in the argument of the exponent leaving the same indexes of phase shifts \( \delta_m \) and \( \delta_{m'} \).

Now inserting the obtained differential cross-section (11.35) into Eq. (11.7) we obtain the total cross-section

\[
\sigma = \frac{4}{E} \sum_{m,m'=-\infty}^{\infty} \delta_{m,m'} e^{i[(\delta_{m'}-\delta_m)]} \sin \delta_m \sin \delta_{m'}, \tag{11.37}
\]

Note the above mentioned change \( m \to -m \) and \( m' \to -m' \) in the exponent argument now appears as the same change in the argument of the Kronecker symbol \( \delta_{m,m'} \). It is evident that this change does not influence the total cross-section, and consequently, it is the same for both \( K \) and \( K' \) valley electrons.

Taking into account Eq. (11.29) the partial cross-section contribution to the total cross-section can be presented as

\[
\sin^2 \delta_m = \frac{[J_m(E) + J_{m+1}(E)]^2}{[J_m(E) + J_{m+1}(E)]^2 + [Y_m(E) + Y_{m+1}(E)]^2}, \tag{11.38}
\]

what enables us to calculate the scattering cross-section directly.
CHAPTER 11. SCATTERING OF DIRAC ELECTRONS BY CIRCULAR MASS BARRIERS: VALLEY FILTER AND RESONANT SCATTERING

Figure 11.2: The energy dependence of the partial sums $\sigma_M$ contributing to the total cross-section. The italic numbers on the curves indicate the number $M$. The black curve for $M = 15$ corresponds to the convergent result.

The energy dependence of the total cross-section where the sum is restricted by the value $M \ (|m| \leq M)$ is shown in Fig. 11.2. We see a rather good convergence at low energies where three terms (i.e. $m = 0, \pm 1$) are already sufficient.

The oscillating behavior of the energy dependence of the partial sum follows from the same behavior of the separate terms in Eq. (11.37) that can be easily explained calculating the asymptotic of the phase shifts. Indeed, using the asymptotic of the Bessel functions and replacing $\Delta_m$ by $\Delta_m |r=1$ we have the following asymptotic expression for the scattering phase (11.29):

$$\tan \delta_m = -\frac{J_m(E) + J_{m+1}(E)}{Y_m(E) + Y_{m+1}(E)} \approx \frac{\cos \Delta_m + \cos \Delta_{m+1}}{\sin \Delta_m + \sin \Delta_{m+1}}$$

$$= \frac{\cos \Delta_m + \sin \Delta_m}{\sin \Delta_m - \cos \Delta_m} = \frac{\sin (\Delta_m + \pi/4)}{\cos (\Delta_m + \pi/4)}$$

$$= -\tan (\Delta_m + \pi/4).$$

Thus, in the asymptotic region we have

$$\sin^2 \delta_m = \sin^2 (E - \pi m/2),$$

what explains the waving behavior of the obtained partial contributions to the total cross-section.
11.5. SCATTERING BY AN IMPENETRABLE CIRCLE

By the way, this simple expression for the scattering phase enables us to perform the approximate summation in Eq. (11.37) for large energies which results in the limit cross-section \( \sigma_{\text{lim}} = 4 \) as can also be seen clearly in Fig. 11.2. This value is twice larger than the classical value \( \sigma_{\text{cl}} = 2 \) that can be obtained assuming that relativistic electrons are moving along trajectories given by non quantum mechanical equations of motion. This discrepancy is caused by the diffraction of the electronic waves when they are scattered by hard wall type potentials, and it is inherent over scattering by small angles. It is remarkable that relativistic electrons exhibit the same feature as Schrödinger electrons (see the textbook [137]).

In Appendix A we present similar results for Schrödinger electrons (see Fig. 11.9). Note that there are some differences in their \( k \)-dependence: 1) in the low energy limit the cross-section of the Schrödinger electrons diverge logarithmically, while for Dirac electrons it becomes zero, and 2) \( \sigma(k) \) for Schrödinger electrons is an uniform decreasing function of \( k \) while for Dirac electrons it exhibits oscillations in the low energy region. Both cross-sections approach the high energy limit from above.

Inserting differential cross-section (11.35) into Eq. (11.8) we obtain the inverse momentum relaxation time (or the dissipative resistivity component)

\[
\gamma = \frac{2}{E} \sum_{m,m'=-\infty}^{\infty} \left[ 2 - \delta_{m',m+1} - \delta_{m',m-1} \right] \\
\times e^{i(\delta_{m'} - \delta_m)} \sin \delta_m \sin \delta_{m'}
\]

(11.41)

By the way the change \( m \rightarrow -m \) and \( m' \rightarrow -m' \) in the arguments of the Kronecker symbol does not influence the value of the above expression. Consequently, the above inverse momentum relaxation time expression is the same for both \( K \) and \( K' \) valley electrons.

Now inserting the phases obtained by solving Eq. (11.29) into Eq. (11.41) we get the result that is shown in Fig. 11.3. It’s behavior is qualitatively similar to the one for the total cross-section. For large energies it approaches the limiting value \( \gamma = 8/3 \), which we obtain by calculating the integral (11.8) with the classical differential cross-section, confirming the known fact that the integral (11.8) is not sensitive to forward scattering. Thus this relaxation time isn’t affected by the above mentioned discrepancy between the quantum and classical result as it was with the total cross-section.

Note that there is an essential difference in the separate contributions to the total cross-section \( \sigma \) and the inverse momentum relaxation time \( \gamma \). The partial
contributions to $\gamma$ do not exhibit any oscillating behavior that was inherent in the case of $\sigma$. This is expected from Eq. (11.39) where the difference of neighboring phases $(\delta_m - \delta_{m+1})$ doesn’t depend on energy in the asymptotic region.

And at last inserting the differential cross-section (11.35) into Eq. (11.9) we obtain the perpendicular (or Hall) component of the conductivity

$$\eta = \frac{-2i}{\pi E} \sum_{m,m'=-\infty}^{\infty} \left[ \delta_{m',m+1} - \delta_{m',m-1} \right] \times e^{i(\delta_{m'} - \delta_m)} \sin \delta_m \sin \delta_{m'}$$

(11.42)

The result is shown in Fig. 11.4. Naively we would expect that $\eta = 0$ at zero magnetic field. To our surprise we find that $\eta < 0$ and that it conserves it’s sign as a function of $E$. It means that the mass barrier acts similar as a magnetic field. In order to obtain the result for $K'$ valley electrons we have to change $m \rightarrow -m$ and $m' \rightarrow -m'$ in the arguments of Kronecker symbols in the first line of Eq. (11.42). It is evident that due to this change the Hall component of the resistivity $\eta$ changes it’s sign. Thus, the electrons from different valleys are deflected to opposite sides.
of the sample. There is no net charge build up across the sample and thus no Hall voltage. But there is a separation of different $K$ and $K'$ valley electrons across the sample and thus we can use this effect for valley filtering purposes.

**11.6 Scattering on a penetrable circle**

Now we turn to our last problem — scattering of Dirac electrons by a penetrable circle in order to demonstrate how possible quasi-bound states reveal themselves in the scattering cross-section. For this purpose we have to solve the Dirac equation for free electrons (11.25) in both $I$ and $III$ regions and to apply boundary conditions (11.19). These solutions are given by Eq. (11.26) for the inner region $I$, and by Eq. (11.28) for the outer region $III$. Moreover, the procedure of the exclusion of the incident exponent is the same as it was performed in Sec. 11.5. Thus we can immediately write down Eqs. (11.34) for the components of the scattering amplitudes, and use the previous expressions for the scattering cross-section (11.35, 11.37, 11.41, 11.42).

The single procedure that should be performed is to satisfy the boundary conditions (11.19) and calculate the phase shifts $\delta_m$. Inserting into Eq. (11.19) the
solutions (11.26) and (11.28) we obtain the set of two equations:

\[
\begin{align*}
C J_{m+1} + S Y_{m+1} - F J_{m+1} &= -P \left\{ C J_m + S Y_m + F J_m \right\}, \quad (11.43a) \\
C J_{m} + S Y_{m} - F J_{m} &= -P \left\{ C J_{m+1} + S Y_{m+1} + F J_{m+1} \right\}, \quad (11.43b)
\end{align*}
\]

where for the sake of shortness we denoted

\[
C = w_m \cos \delta_m, \quad S = w_m \sin \delta_m, \quad (11.44)
\]

and omitted the arguments \(E\) of all Bessel functions.

Now excluding coefficient \(F\) we obtain a single equation. It can be solved for the tangent of the phase shift, and using the expression for the Wronskian of the Bessel functions we arrive at

\[
\tan \delta_m = -\frac{(J_{m+1} + J_{m})(J_{m} - J_{m+1})}{(Y_{m+1} + Y_{m})(J_{m} - J_{m+1}) - 1/p E}, \quad (11.45)
\]

where the symbol

\[
p = \frac{\pi P}{(1 - P)^2} \quad (11.46)
\]

characterizes the impenetrability of the circle. The value \(p = \infty\) corresponds to a completely impenetrable circle, i.e. the previously considered scattering on an impenetrable anti-dot, while the value \(p = 0\) corresponds to the case of complete penetration, or the absence of any scatterer.

The numerical results for the lowest contribution \((m = 0)\) to the total cross-section are shown in Fig. 11.5 for different \(p\) values. The vertical lines indicate the energies of the bound states of the dot obtained by solving Eq. (11.27) as described in Sec. 11.4. Although now the dot is penetrable and it has no bound states, the corresponding quasi-bound states reveal themselves as narrow gaps close to the maxima of the oscillating partial contribution. Note that this is a particular feature of Dirac electrons. While in the case of Schrödinger electrons the quasi-bound states appear as peaks in the cross-section (see Figs. 11.10 and 11.11 in Appendix A).

According to Eq. (11.45) it seems that there should be one more set of gaps in the partial cross-section, related to the equation

\[
J_m(E) + J_{m+1}(E) = 0. \quad (11.47)
\]

But in this case, however, after neglecting the last term in the denominator of Eq. (11.45) it coincides with the phase (11.29) obtained for the scattering by the
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Figure 11.5: The partial $\sigma_0$ contribution to the total cross-section for different values of the penetrable parameter $p$ of the circular scatterer. The curve marked by $p = \infty$ corresponds to the case of scattering by an impenetrable circle.

impenetrable circle, and in such a way it indicates that the above condition defines the flat minimum related to the diffraction pattern in the cross-section considered in Sec. 11.5.

These gaps in the partial cross-section reveal themselves in the total cross-section as shown in Fig. 11.6. Because of the contribution of the other partial waves the gaps no longer reach zero as e. g. shown in the case of the partial cross-section $\sigma_0$. Notice that they become more pronounced and narrower when the parameter $p$ increases (when the circle becomes less penetrable).

In Fig. 11.7 the results for the inverse momentum relaxation time and in Fig. 11.8 those for the perpendicular component of the resistivity are presented.

We see that although Eqs. (11.41) and (11.42) are more sophisticated functions of the phases $\delta_m$ and even two neighboring phases $\delta_m$ and $\delta_{m+1}$ are intermixed, nevertheless the resonant behavior, i.e. the negative peaks, is still clearly visible in the inverse momentum relaxation time. The behavior of peaks in the Hall component of the resistivity, however, is more complicated, and exhibits both sharp peaks and dips where now the sign of $\eta$ can change in small regions of energy.
Figure 11.6: The total cross-section $\sigma$ for a penetrable circular scatterer for different $p$ values. The curve marked by $p = \infty$ corresponds to the case of scattering on an impenetrable circle.

11.7 Conclusions

We investigated the scattering of Dirac electrons by sharp circular mass barriers, where we studied both hard wall type anti-dot and circular penetrable scatterer. For this purpose the proper boundary conditions for Dirac equation were derived, and it was illustrated how it is possible to use formally $\delta$-type functions describing relativistic systems with high and sharp potentials.

The differential and total cross-section, the inverse momentum relaxation time and the perpendicular (Hall) component of resistivity were calculated. The obtained results were compared with analogous results for scattering of Schrödinger electrons by similar scatterers.

It was shown that the scattering of Dirac electrons even by azimuthal symmetric structures depends on the valley index: the $K$ valley electrons are preferentially deflected to one side (the Hall component of the resistivity isn’t zero) while the electrons of the other $K'$ valley are deflected to the other side of the sample. This enables one to use this property for valley index filtering in transport experiments.

There is an essential difference in the energy dependence of the cross-section between Dirac and Schrödinger electrons. At small energies the cross-section for Dirac electrons tend to zero while those for Schrödinger electrons diverge logarith-
11.7. CONCLUSIONS

Figure 11.7: The inverse momentum relaxation time calculated according Eq. (11.41) for a penetrable circular scatterer.

Figure 11.8: The Hall component $\eta$ calculated according Eq. (11.42) for a penetrable circular scatterer.

mically. This feature of Dirac electron is caused by the fact that zero energy for Dirac electron actually corresponds to the middle of the half-filled band, and not to the bottom of it as in the Schrödinger electron case.

We showed that in the case of Dirac electron scattering on a penetrable circle
the quasi-bound states reveal themselves as sharp gaps in the total cross-section, the inverse momentum relaxation time and the Hall component of the resistivity as well. In the case of Schrödinger electrons those resonances show up as peaks in the cross-sections, and thus their appearance is qualitatively very different.

11.8 Appendix:

11.8.1 Scattering of a Schrödinger electron by circular barriers

In this Appendix we study the scattering of Schrödinger electrons by sharp circular potentials shown in Fig. 11.1. This allows us to compare them with results for Dirac electrons considered in the present paper.

Here scattering is now described by the single component wave function $\Psi(r)$ satisfying the stationary Schrödinger equation

$$(\nabla^2 + k^2)\Psi(r) = 0,$$

where the symbol $k$ stands for the electron momentum related to it's energy as $E = k^2/2$. Now we use dimensionless units defined as follows. The coordinates will be measured in the radius of the circular scatterer $R$, energy — in $\hbar^2/mR^2$ units, and the electron momentum — in $\hbar/R$ units.

In polar coordinates the wave function $\Psi(r)$ is usually expanded into a Fourier series like $U(r)$ component of Dirac function in Eq. (11.12) with radial components $\psi_m(r)$ satisfying the Bessel equation. That is why all mathematics is practically the same as used in previous sections with a single replacement of the Dirac electron energy $E$ by the momentum $k$ of the Schrödinger electron. Consequently, we obtain the same differential cross-section given by Eq. (11.35), and Eqs. (11.37) and (11.41) for the total cross-section and inverse momentum relaxation time.

Nevertheless, there is an essential difference between Dirac and Schrödinger electrons which is the different boundary conditions that will lead to different scattering phases.

Thus, in the case of scattering on a circular hard wall potential (see Fig. 11.1(a)) every radial component of the wave function has to satisfy the zero boundary condition

$$\psi_m(1) = 0,$$

what leads to the following equation for the phase

$$\tan \delta_m = -\frac{J_m(ka)}{Y_m(ka)},$$
instead of Eq. (11.29) for the Dirac electron. The partial contributions and the total cross-section calculated by using the above phase equation are shown in Fig. 11.9.

Figure 11.9: The energy dependence of the partial sums $\sigma_M$ contributing to the total cross-section for Schrödinger electrons. The italic numbers on the curves indicate the number $M$.

In the case of an extremely narrow penetrable circle, i.e. a $\delta$-type potential, Eq. (11.48) has to be replaced by
\[
\left\{ \nabla^2 + k^2 - p\delta(r - 1) \right\} \psi(r) = 0
\]  
(11.51)
what leads to the following boundary conditions for the radial wave function components on the circle:
\[
\psi_m(1 + 0) = \psi_m(1 - 0), \quad \tag{11.52a}
\]
\[
\psi'_m(1 + 0) - \psi'_m(1 - 0) = p\psi_m(1). \quad \tag{11.52b}
\]
This leads to the following scattering phase equation:
\[
\tan \delta_m = -\frac{J_m(k)}{Y_m(k) - 2/p\pi J_m(k)}.
\]  
(11.53)
From it we obtain the following partial contribution to the total cross-section:
\[
\frac{4}{k^2} \sin^2 \delta_m = \frac{4J_m^2(k)}{k \{ J_m^2(k) + [Y_m(k) - 2/p\pi J_m(k)]^2 \}}.
\]  
(11.54)
Figure 11.10: The $m = 0$ contribution to the total cross-section for Schrödinger electrons scattered on penetrable circular potentials, shown by red solid curve. Green dotted curve is the envelop function $4/k$, and the blue dashed curve is the result for scattering on impenetrable scatterers.

The typical contribution (when $m = 0$) is shown in Fig. 11.10 by red solid curve. Narrow peaks appear close to the positions of the bound states of a dot that are defined by the equation $J_m(k) = 0$. This can be also seen from Eq. (11.54) which formally is similar to a Lorentzian curve. The top of the peak is achieved when the second term in the denominator (the analog of detuning) in Eq. (11.54) is zero. In the case of small penetrability of the scatterer this can be realized if the large parameter $p \gg 1$ is compensated by a small $J_m(k) \ll 1$ value. But then the contribution becomes equal to $4/k$ what indicates that the maximum of all peaks reach the above envelope function shown by green dotted curve in Fig. 11.10. One more property of the partial contribution follows from the fact that it is rather close to the same contribution in the case of scattering by impenetrable scatterer shown by the blue dashed curve (Eq. (11.53) converts itself into Eq. (11.50) when $p = \infty$) what indicates that the peaks appear at the minima of that dashed curve.

These resonances show up also in the total cross-section as seen in Fig. 11.11. The comparison with the blue dashed curve calculated for $p = \infty$ indicates clearly that the quasi-bound states appear in the total cross-section as positive peaks.
Figure 11.11: The same as Fig. 11.10 but now for the total cross-section.
Scattering of Dirac electrons by magnetic fluxes

Abstract. The scattering of two-dimensional (2D) massless electrons is investigated in the presence of a random array of circular magnetic flux tubes. We derived the momentum relaxation time and the Hall factor using optical theorem techniques for scattering. Electrons with energy close to those of the Landau levels in the flux tubes have longer lifetime inside the magnetic flux tube which show up as sharp structures in the Hall factor and the magneto-resistance.

12.1 Introduction

Scattering by a magnetic flux tube was analyzed many years ago by Y. Aharonov and D. Bohm [138]. Such a magnetic flux introduces a phase factor which ultimately results in the Aharonov-Bohm (AB) effect. They pointed out that due to the very slow decrease of the vector potential at infinity, it results in a slow convergence of the cross-section expansion into series of angular momentum and to a non-analytical behavior.

The Aharonov-Bohm effect is a purely quantum mechanic effect which was first verified experimentally by R. G. Chamberes in 1960 [139]. Such a magnetic flux tube can be realized by having a magnetic vortex piercing the graphene layer or by covering graphene with a type I superconductor with a circular hole. Another way is by deforming the lattice locally; this results in local strain which in graphene can induce an effective inhomogeneous magnetic field [69, 108].

Previously such flux tubes was introduced as external scatters in a normal 2D electron gas (2DEG) system. Experimentally this can be realized by depositing a thin superconducting film above the 2D layer (with an intermediate thin insulator to prevent electrical contact). In an applied perpendicular magnetic field and for temperatures below the superconducting critical temperature the field is broken up into vortex lines each carrying a flux quantum $\phi_0 = \hbar c/2e$. For low magnetic fields: i)
the flux lines are well separated and the magnetic field are confined to small circular areas in the 2D layer, and i) the position of the flux lines are random due to the presence of inhomogeneities in the superconducting film. These flux lines act as magnetic scatters for the charge carriers in the 2D layer and the concentration of these scatterers can be tuned by the strength of the magnetic field. Such a system was previously studied experimentally [140–142] and theoretically [126, 143] for a non-relativistic 2D electron gas. The Hall resistance and the magnetoresistance was measured where a suppression of the Hall resistance below the classical result was found at low magnetic field.

In the present paper we investigate the system of graphene with on top a superconducting film. Now relativistic electrons will scatter on the flux tubes that are piercing through graphene. And because electrons in graphene have zero energy Landau level, we are expecting different scattering behaviors as compared to the previously studied 2DEG counterpart.

The standard procedure for solving the electron scattering problem is based on the division of its wave function into two parts. The first part is the incident unperturbed plane wave and the second one describes the radial flow of the scattered electrons. In the case of isotropic scatterer both of them are presented as Fourier expansions in azimuthal harmonics, and the differential cross-section is obtained by calculating the corresponding partial radial flows.

This procedure becomes problematic in the case of magnetic scattering due to the slow decay of the vector potential at infinity. As a consequence the incoming exponent has to be corrected by a phase factor that finally leads to non-analytic behavior of the scattered part spoiling its convergence. Therefore we propose another procedure to obtain the momentum relaxation time evading the above complication.

### 12.2 Scattering of 2D Dirac electrons

In order to illustrate our method to calculate the scattering cross-section we consider the simplest problem of scattering of Dirac electrons by a circular hole made in an infinite sheet of graphene. The layout of the system is shown in Fig. 12.1. We measure all distances in units of the radius of the hole. That is why in Fig. 12.1 the radius of the hole $R$ is equal to unity.

We assume that the homogeneous flow of electrons is coming from $-\infty$ along the $x$-axis, and calculate the probability for them to be scattered and deflected by an angle $\varphi$.

The mathematical model is based on the stationary Dirac equation $\{H - E\} \Psi(r) =$
0 with the dimensionless Hamiltonian
\[
H = \sigma \cdot \mathbf{p} = \begin{pmatrix} 0 & -i\{\partial/\partial x - i\partial/\partial y}\ 
-\{\partial/\partial x + i\partial/\partial y\} \\
0 & 0 \end{pmatrix},
\]
(12.1)
where the velocity is measured in \(v_F\) (Fermi velocity) units and the energy in \(\hbar v_F/R\) units.

The wave function consists of two components
\[
\Psi(r) = \begin{pmatrix} A(r) \\
B(r) \end{pmatrix},
\]
(12.2)
The electron density and current are
\[
\rho = \Psi^+ \Psi, \quad J = \Psi^+ \mathbf{\sigma} \Psi.
\]
(12.3)
The wave function of the free electron propagating along the \(x\)-axis (towards \(+\infty\)) is as follows:
\[
\Psi_0(r) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\
1 \end{pmatrix} e^{ikx},
\]
(12.4)
with \(k > 0\). It describes a homogeneous electron flow with density \(\rho = 1\), and current \(J = \{1, 0\}\).

In standard scattering theory the wave function far away from the scatterer is given by
\[
\Psi(r) \approx \Psi_0(r) + \frac{f(\phi)}{\sqrt{r}} e^{ikr}.
\]
(12.5)
The scattering amplitude is now composed of two components:
\[
f = \begin{pmatrix} a \\
b \end{pmatrix}.
\]
(12.6)
Having in mind the definition of the current we define the differential cross-section as follows:

$$d\sigma(\varphi) = P(\varphi)d\varphi = f^+(\varphi)(\mathbf{\sigma} \cdot \mathbf{n})f(\varphi)d\varphi.$$  \hspace{1cm} (12.7)

Here symbol \( \mathbf{n} \) stands for the unit vector perpendicular to the above mentioned circle, having the following components \( n_x = r \cos \varphi, \quad n_y = r \sin \varphi \). Consequently,

$$\left( \mathbf{\sigma} \cdot \mathbf{n} \right) = \left( \begin{array}{cc} 0 & e^{-i\varphi} \\ e^{i\varphi} & 0 \end{array} \right),$$  \hspace{1cm} (12.8)

and the differential cross-section reads

$$P(\varphi) = e^{i\varphi}ab^* + e^{-i\varphi}a^*b.$$  \hspace{1cm} (12.9)

The presence of the hole inside the graphene sheet will be taken into account by the boundary condition on the perimeter of it (on the circle \( r^2 = 1 \)). Actually graphene isn’t an isotropic material, and the boundary condition depends on the angle \( \varphi \). In order to implement this boundary condition we have to go back to the discrete problem and investigate the equations within the tight binding approximation. The equations on the border (on the hole perimeter) are different as compared with the equations in the plane. They lead to an additional relation between the \( A \) and \( B \) components of the wave function on the border. In order not to complicate the scattering problem we assume the most simple relation, namely,

$$A(r)\bigg|_{r=1} = 0.$$  \hspace{1cm} (12.10)

describing the zig-zag boundary conditions.

Making use of the circular symmetry we have the following angular wave function dependence:

$$\begin{pmatrix} A(r, \varphi) \\ B(r, \varphi) \end{pmatrix} = e^{i\varphi} \begin{pmatrix} a(r) \\ e^{i\varphi}b(r) \end{pmatrix},$$  \hspace{1cm} (12.11)

and the Dirac equation reduces to the following set of coupled ordinary differential equations for the radial wave function components

$$\begin{cases} \frac{d}{dr} + \frac{m+1}{r} & b = Ea, \\ -\left( \frac{d}{dr} - \frac{m}{r} \right) a = Eb. \end{cases}$$  \hspace{1cm} (12.12a, b)

We transform the two differential equations of first order into a single equation of second order:

$$\left\{ \frac{1}{r} \frac{d}{dr}r - \frac{m^2}{r^2} + k^2 \right\} a = 0.$$  \hspace{1cm} (12.13)
12.2. SCATTERING OF 2D DIRAC ELECTRONS

where \( k = |E| \). We assume that \( k > 0 \) and \( E > 0 \), and thus \( k = E \).

The solution of the above equation is a linear combination of Bessel functions

\[
a(r) = w_n \{ \cos \delta_m \cdot J_m(kr) + \sin \delta_m \cdot Y_m(kr) \}.
\]

(12.14)

Now using Eq. (12.12b) we obtain the second component of the eigenfunction:

\[
b = -\frac{1}{E} \left\{ \frac{d}{dr} - \frac{m}{r} \right\} a
\]

\[
= w_n \{ \cos \delta_m \cdot J_{m+1}(kr) + \sin \delta_m \cdot Y_{m+1}(kr) \}.
\]

(12.15)

Thus we have the following expansion for wave function components:

\[
A(r, \varphi) = \sum_{m=-\infty}^{\infty} e^{im\varphi} \cdot w_n \times \{ \cos \delta_m \cdot J_m(kr) + \sin \delta_m \cdot Y_m(kr) \}.
\]

(12.16)

\[
B(r, \varphi) = i \sum_{m=-\infty}^{\infty} e^{i(m+1)\varphi} \cdot w_n \times \{ \cos \delta_m \cdot J_{m+1}(kr) + \sin \delta_m \cdot Y_{m+1}(kr) \}.
\]

(12.17)

The coefficients \( w_n \) and \( \delta_m \) are determined by the boundary condition on the hole perimeter (on the circle \( r = 1 \)) and the wave function asymptotic (12.4).

In the asymptotic region \((r \to \infty)\) we use the following Bessel function expressions:

\[
J_m(kr) = \sqrt{\frac{2}{\pi kr}} \cos \Delta_m,
\]

(12.18a)

\[
Y_m(kr) = \sqrt{\frac{2}{\pi kr}} \sin \Delta_m,
\]

(12.18b)

\[
\Delta_m = kr - \frac{\pi}{2} m - \frac{\pi}{4}.
\]

(12.18c)

It enables to present Eqs. (12.16) and (12.17) in the asymptotic region as

\[
A(r) = \sqrt{\frac{2}{\pi kr}} \sum_{m=-\infty}^{\infty} w_n e^{im\varphi} \cos(\Delta_m - \delta_m),
\]

(12.19)

\[
B(r) = i \sqrt{\frac{2}{\pi kr}} \sum_{m=-\infty}^{\infty} w_n e^{i(m+1)\varphi} \cos(\Delta_{m+1} - \delta_m).
\]

(12.20)
CHAPTER 12. SCATTERING OF DIRAC ELECTRONS BY MAGNETIC FLUXES

So, we have to put these expansions into agreement with the asymptotic (12.4). For this purpose we shall present the exponent in Eq. (12.19) as

\[ e^{ikx} = e^{ikr \cos \varphi} = \sum_{m=\infty}^{\infty} i^m e^{im\varphi} J_m(kr) \]

\[ \approx \sqrt{\frac{2}{\pi kr}} \sum_{m=\infty}^{\infty} i^m e^{im\varphi} \cos \Delta_m \]

\[ = \sqrt{\frac{1}{2\pi kr}} \sum_{m=\infty}^{\infty} i^m e^{im\varphi} (e^{i\Delta_m} + e^{-i\Delta_m}) . \] 

(12.21)

Rewriting the asymptotic of this component of Eq. (12.19) as

\[ A(r) = \sqrt{\frac{1}{2\pi kr}} \sum_{m=\infty}^{\infty} w_m e^{im\varphi} \left\{ e^{i(\Delta_m - \delta_m)} + e^{-i(\Delta_m - \delta_m)} \right\} . \]

(12.22)

The phases \( \delta_m \) follow from the boundary condition Eq. (12.10) applied for every radial component:

\[ \tan \delta_m = - \frac{J_m(k)}{N_m(k)} . \]

(12.23)

The coefficients of the exponents in Eq. (12.22) representing the incoming wave (the second terms in parenthesis and braces) have to be equal. Thus, we have to assume that

\[ w_m = i^m e^{-i\delta_m} . \]

(12.24)

This result into the following expressions for the components of the scattering amplitude (12.6):

\[ a = e^{-i\pi/4} \sqrt{\frac{1}{2\pi k}} \sum_{m=\infty}^{\infty} e^{im\varphi} \left\{ e^{-2i\delta_m} - 1 \right\} , \]

(12.25a)

\[ b = e^{-i\pi/4} \sqrt{\frac{1}{2\pi k}} \sum_{m=\infty}^{\infty} e^{im\varphi} \left\{ e^{-2i\delta_{m-1}} - 1 \right\} , \]

(12.25b)

and finally the differential cross-section (12.9):

\[ P(\varphi) = \frac{4}{\pi k} \sum_{m,m'=\infty}^{\infty} e^{i(m-m')\varphi-(\delta_m - \delta_{m'})} \sin \delta_m \sin \delta_{m'} . \]

(12.26)
We are interested in the reciprocal momentum relaxation time:

\[ \gamma \equiv \frac{1}{\tau} = k \int_0^{2\pi} d\varphi (1 - \cos \varphi) \sigma(\varphi) \]

\[ = 4 \sum_{m=-\infty}^{\infty} \sin^2 (\delta_m - \delta_{m+1}), \quad (12.27) \]

that characterizes the effectiveness of electron momentum scattering, and its density related to the mobility of the electrons. Notice that the pre-factor is a factor 2 different from the case of normal electrons scattered by a 2D hard wall sphere.

We draw your attention to the important point that these Fourier expansions are not correctly defined. Note that the incident radial flow reads

\[ \tilde{J}_0 = r(e^{-i\varphi} A_0 B_0^* + e^{i\varphi} A_0 B_0^*). \quad (12.28) \]

After substituting \( A_0 \) and \( B_0 \) we find

\[ \tilde{J}_0 = \frac{2i}{\pi k} \sum_{m,m'=-\infty}^{\infty} e^{i(m' - m)(\varphi + \pi/2)} \sin \left( (m' - m) \frac{\pi}{2} \right) \]

\[ = \frac{1}{k} \left[ 2\delta(\varphi + \pi) - 2\delta(\varphi) \right] \sum_{m} 1, \quad (12.29) \]

which is divergent. The reason is that the exponent at infinity is expanded into series of radial functions with \( 1/r \) asymptotic which is responsible for the convergence problem. Moreover, the asymptotic of Bessel functions is valid only in the region where \( kr \gg n \). The invalid \( 1/r \) type asymptotic is formally compensated by the divergent sum of unities. In spite of this ill posed problem the compensation of the incident flow in the total wave function is carried out in every separate term, after which the summation is performed leading to a finite result.

Nevertheless the above procedure is useful as it prompts that when calculating the momentum relaxation time only the incoming part of the incident wave expansion (proportional to \( \delta(\varphi + \pi) \)) has to be eliminated from the total electron flow.

Now we shall show how to obtain the final result i. e. Eq. (12.27), using the radial flows directly and avoiding the separation of the wave function division given
by Eq. (12.5). It is evident that the radial flow of scattered electrons can be presented as

\[ J_s = J - J_0 - J_c, \]  

(12.30)

where \( J \) is the total radial flow calculated by means of the total wave function given by Eqs. (12.19) and (12.20), \( J_0 \) is the Fourier expansion of the incident flow given by Eq. (12.21). The last term represents the flow corresponding to the interference of incident and scattered waves. The formal calculation of it using Eqs. (12.19), (12.20) and (12.21) gives the following result:

\[ J_c (\varphi) = e^{-i \varphi} (A_s \ast B_s + A_s \ast B_1) + e^{i \varphi} (A_s B_1^* + A_1 B_s^*) \]

(12.31)

Thus it reduces the incident flow according to the so called optical theorem. It is important for us, however, that this flow is proportional to \( \delta(\varphi) \), and consequently, gives no contribution to the integral (12.27) that we have to calculate. For the same reason the first term in the Fourier expansion of the incident exponent given by Eq. (12.21) is not important. Thus, the effective cross-section suitable for momentum relaxation calculation can be presented as

\[ \tilde{\sigma}(\varphi) = \frac{1}{\pi k} \left\{ r J + \frac{1}{\pi} \sum_{m, m'}^{\infty} e^{i(m-m')(\varphi + \pi)} \right\}. \]  

(12.32)

So, using Eqs. (12.19) and (12.20) we calculate the total radial flow:

\[ J = \frac{2i}{\pi k} \sum_{m, m'}^{\infty} e^{i(m-m')(\varphi + \pi/2)} e^{i(\delta_m - \delta_{m'})} \times \sin [(m - m') \pi/2 + (\delta_m - \delta_{m'})]. \]  

(12.33)

Comparing the obtained result with Eq. (12.29) we see that in order to compensate the incoming flow we have to choose the coefficients according to Eq. (12.24). Then the chosen effective cross-section Eq. (12.32) becomes

\[ \tilde{\sigma}(\varphi) = \frac{1}{\pi k} \sum_{m, m'}^{\infty} e^{i(m-m') \varphi} e^{2i(\delta_m - \delta_{m'})}. \]  

(12.34)

At last substituting it into integral (12.27) we obtain the following reciprocal mo-
12.3. SCATTERING BY MAGNETIC FLUX TUBES

momentum relaxation time:

\[ \gamma = \sum_{m,m'=-\infty}^{\infty} e^{2i(\delta_m - \delta_m')} \left[ 2\delta_{m,m' + 1} - \delta_{m,m' - 1} \right] \]

\[ = \sum_{m=-\infty}^{\infty} \left[ 2 - e^{2i(\delta_{m+1} - \delta_m)} - e^{2i(\delta_m - \delta_{m+1})} \right] \]

\[ = 4 \sum_{m=-\infty}^{\infty} \sin^2(\delta_m - \delta_{m+1}) \] (12.35)

Using trigonometric equalities it is easy to prove that it coincides with Eq. (12.27). This confirms the correctness of the proposed method of calculation.

![Figure 12.2: Azimuthal vector potential component \( A_\phi \) (black solid curve), and perpendicular magnetic field component \( B_z \) (gray dashed curve).](image)

12.3 Scattering by magnetic flux tubes

Now let us consider the analogous scattering problem which is shown in Fig. 12.2, where we have a magnetic field \( B \) inside the circle \((r \leq r_0)\) and no magnetic field outside it. This is a simple model system for a magnetic flux as found in e. g. a type II superconductor. We define the dimensionless variables as \( r \rightarrow \ell_B r \) with \( \ell_B = \sqrt{\hbar c/ eB} \), \( v \rightarrow v_F v \) (\( v_F \) the Fermi velocity), \( E \rightarrow E_0 E \) with \( E_0 \rightarrow \hbar v_F / \ell_B \), the magnetic flux \( \phi \rightarrow \phi_0 \phi \) with \( \phi_0 = h/e \) and relaxation time \( \gamma \rightarrow \gamma_0 \gamma \) with \( \gamma_0 = (1/4\pi^2)(n_0/n_e)(h/e^2) \) where \( n_e \) is the electron concentration, \( n_0 \) the concentration of magnetic flux tubes. The corresponding vector potential for \( B(r) = B_0 \Theta(r - r_0) \) in the symmetric gauge has only an angular component,

\[ A_\phi(r) \equiv \begin{cases} -y/x, & r \leq r_0; \\ r_0^2/r, & r_0 < r \end{cases} \] (12.36)
Figure 12.3: (a) The reciprocal momentum relaxation time ($\gamma = 1/\tau$) and (b) the Hall factor $F_H$ for different flux radius $r_0 = 3, 3.5, 4.5$ and $5$. The vertical dotted lines indicate the position of the Landau levels in case of a homogenous magnetic field.

The momentum operator $p$ in Eq. (12.1) should be replaced by $p + A$. The solution in the inner region ($r < r_0$) for the wave function $b$ component can be presented as

$$b_-(r) = Ar^{m+1}e^{-r^2/4}F(a, b, z),$$

where $F(a, b, z)$ is the confluent hypergeometric (Kummer) function, and $a = (|m + 1| + m + 1 - E)/2$, $b = |m + 1| + 1$ and $z = r^2/2$. The solution outside the circle ($r > r_0$) reads as

$$b_+(r) = \cos \delta_m J_{|m+1+\alpha|}(r|E|) + \sin \delta_m Y_{|m+1+\alpha|}(r|E|),$$

with $\alpha = r_0^2/2$. The component $a$ follows from Eq. (12.12a):

$$a_\pm(r) = \frac{1}{E} \left\{ \frac{d}{dr} + g(r) + \frac{m + 1}{r} \right\} b_\pm(r).$$
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Figure 12.4: (a) The reciprocal momentum relaxation time ($\gamma = 1/\tau$) and (b) the contribution of the AB effect to the reciprocal momentum relaxation time $\gamma_{AB}$ as a function of magnetic flux ($\phi/\phi_0 = \alpha$) for different values of the Fermi energy.

where

$$g(r) = \begin{cases} r, & 0 < r < r_0; \\ \frac{r_0^2}{r}, & r_0 < r < \infty. \end{cases}$$

(12.40)

In the outer region we find explicitly

$$a_+(r) = \frac{|E|}{E} \left\{ \cos \delta_m J_{\nu-1}(z) + \sin \delta_m Y_{\nu-1}(z) \right\},$$

(12.41)

where $\nu = |m + 1 + \alpha|$, and $z = |E|r$. These components obey the following boundary conditions at the point $r = r_0$: $a_- = a_+$ and $b_- = b_+$. from which we obtain the phase $\delta_{m+1}$ as

$$\tan \delta_{m+1} = \frac{|E|J_{|m+1+\alpha|}\Phi_m - \Phi_m\Phi_{m+1+\alpha}}{\Phi_m Y_{|m+1+\alpha|} - [E]Y_{|m+1+\alpha|}\Phi_m},$$

(12.42)
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Figure 12.5: Hall factor \((F_H)\) and (b) the contribution of AB effect to the Hall factor \(F_{AB}\) as a function of magnetic flux \((\phi/\phi_0 = \alpha)\) for different values of the Fermi energies.

Here

\[
\Phi_m(r_0) = r_0^{m+1} e^{-r^2/4} F(a, b, r_0^2/2)
\]

(12.43)

The components of \(\Psi(r, \varphi)\) for \(r \to \infty\) can be written as

\[
A = \sqrt{\frac{2}{\pi k r}} \sum_m e^{i(m+1)\varphi} e^{-i(m-1)\pi/2} e^{-i\delta_m} \sin \lambda
\]

(12.44)

with \(k = |E|\), \(\Delta_{\nu - 1} = kr - (\nu - 1)\frac{\pi}{2} - \frac{\pi}{4} - \delta_m\), \(\lambda_{\nu} = \Delta_{\nu} - \delta_m\) and \(\nu = |m + \alpha + 1|\). For the second component we have

\[
B = \sqrt{\frac{2}{\pi k r}} \sum_m e^{i(m+1)\varphi} e^{im\pi} e^{-i\nu\pi/2} e^{-i\delta_m} \cos \lambda_{\nu}
\]

(12.45)
12.3. SCATTERING BY MAGNETIC FLUX TUBES

Following the method described in sec. 12.2 we can calculate \( \tilde{\sigma}(\varphi) \) as

\[
\sigma(\varphi) \rightarrow \tilde{\sigma}(\varphi) = \tilde{J} + \frac{1}{\pi k} \sum_{m,m'} e^{i(m'-m)(\varphi+\pi)}
\]

(12.46)

with \( \tilde{J} = rJ = r(e^{-i\varphi}A^*B + e^{i\varphi}AB^*) \). After some algebra we find

\[
\tilde{\sigma}(\varphi) = \frac{1}{\pi k} \sum_{m,m'=-\infty}^{\infty} e^{i(m'-m)(\varphi+\pi)}
\]

\[\times e^{i\pi(|m'+\alpha+1|-|m+\alpha+1|)} e^{2i(\delta_m - \delta_{m'})},\]

(12.47)

and the reciprocal momentum relaxation time becomes

\[
\gamma \equiv \frac{1}{\tau} = k \int_{0}^{2\pi} \tilde{\sigma}(\varphi)(1 - \cos \varphi) d\varphi
\]

\[= 2 \sum_{m=-\infty}^{\infty} \{1 - \cos(\pi + \lambda_{m+1} - \lambda_m)\},\]

(12.48)

with \( \lambda_m = \pi|m + \alpha| + 2\delta_m \). The momentum relaxation time can be split into two parts

\[
\left(\frac{1}{\tau}\right)_I = 4 \sum_{m=-\infty}^{\infty} \sin^2(\delta_{m+1} - \delta_m),
\]

(12.49)

with the Aharonov-Bohm contribution:

\[
\left(\frac{1}{\tau}\right)_II = 4 \sin^2[\pi(m_0 + \alpha) + \delta_{m_0+1} - \delta_{m_0}]\]

(12.50)

where \( m_0 \) is chosen such that \(-1 < m_0 + \alpha < 0\) \( (m_0 = \text{Int}(-\alpha)) \). This second term is related to the Aharonov-Bohm effect. This is confirmed by considering the limiting case \( r_0 \to 0 \) as done in Ref. [138]. In this case it follows from Eq. (12.42) that \( \delta_m = 0 \) for all \( m \), and the relaxation time involves only the second term

\[
\frac{1}{\tau_{AB}} = 4 \sin^2[(m_0 + \alpha)\pi].
\]

(12.51)

The Hall factor is given by,

\[
F_H = k \int_{0}^{2\pi} \tilde{\sigma}(\varphi) \sin \varphi d\varphi
\]

\[= 2 \sum_{m=-\infty}^{\infty} \sin (\pi + \lambda_{m+1} - \lambda_m).
\]

(12.52)
Similar as for the reciprocal momentum relaxation time we can divide this result into

\[ (F_H)_I = 2 \sum_{m=-\infty}^{\infty} \sin[2(\delta_{m+1} - \delta_m)], \quad (12.53) \]

and an Aharonov-Bohm contribution

\[ (F_H)_{II} = 2 \sin[2\pi(m_0 + \alpha) + 2(\delta_{m+1} - \delta_m)]. \quad (12.54) \]

In the limiting case when the radius of magnetic flux goes to zero we have

\[ F_{AB}^H = 2 \sin[2\pi(m_0 + \alpha)] \quad (12.55) \]

From Eqs. (12.51) and (12.55) when \( \alpha = n \) is an integer the AB contribution in the relaxation time is zero. When \( \alpha \) is half an integer or integer the AB part of the Hall factor is zero. The numerical result for the reciprocal momentum relaxation time and the Hall factor are shown in Figs. 12.3(a) and (b) respectively for two different radius and as function of Fermi energy \( E_F \). The dotted vertical lines show the positions of the Landau levels

\[ E_n = \sqrt{2n + |m + 1| + m + 1}. \quad (12.56) \]

The resonances in Figs. 12.3(a) and (b) correspond clearly with these Landau levels. Same as for the standard electron case [126] when the electron has an energy close to the Landau levels the electron stays longer inside the magnetic vortex. The sawtooth behavior for the Hall factor comes from the fact that the long life time of the electron inside the vortex causes the electron to lose information about the direction of incoming wave and every time a different channel is opened.

In the limiting case when \( E \to 0 \) is small the phase factor \( \delta_m \) from Eq. (12.42) goes to zero and the AB contribution of the total relaxation time and Hall factor become Eq. (12.51) and Eq. (12.55), respectively and we see an oscillatory behavior in Figs. 12.4(a) and 12.5(a) for small energy \( E = 0.01 \).

### 12.4 Conclusions

We evaluate the Hall factor and the momentum relaxation time through magnetic flux tube.

Close to the Landau levels there is a long life time for the electron inside the vortex tube and scattered electron will stay longer inside the vortex and so close to LL we see peaks in relaxation momentum time and also in Hall factor (see Figs. 12.3 (a) and (b)).
12.4. CONCLUSIONS

We also evaluated the Hall factor and momentum relaxation time as a function of magnetic field for different energies. Close to zero energy we have oscillatory behavior for Hall factor and relaxation time. We also plotted the contribution of Aharonov-Bohm to Hall factor and relaxation time separately.
Summary and outlook

Summary of the results

The following new results were obtained in this thesis:

- Using the analogy with optical beams we demonstrated that this is an elegant technique which is also able to provide accurate solutions for the Dirac equation. When considering the transmission of a Dirac electron beam through a single p-n interface we showed that, although a p-n-interface in graphene exhibits a negative refraction for an electron beam, like in an optical metamaterial, it doesn’t influence the electron beam waist which is the essential feature of any lens focusing of optical rays. A contraction of the beam waist, however, is possible if one uses a bent p-n-interface which actually resembles a real lens. Applying periodic potential barriers composed of alternating p-n and n-p interfaces we showed that collimation is possible for a large sub-lattice constant and small barrier heights.

- We showed that a potential barrier in graphene, notwithstanding the Klein effect can act as a Fabry-Perot interferometer where the steps (interfaces) play the role of two parallel mirrors. We showed that in the presence of a perpendicular magnetic field the Fabry-Perot resonances shift linearly with increasing magnetic field.

- Applying an inhomogeneous magnetic field such as a magnetic barrier realized through e.g. the use of a ferromagnetic strip we found that: the transmission probability is angular dependent and one can control this probability by changing the size of the barrier or the magnetic field strength. We showed that such magnetic barrier can act as an electron wave filter. We also showed that in the presence of a superlattice of magnetic barriers we can open a gap in the electron spectrum. These results were extended to bilayer graphene where we obtained quantitatively similar behavior.
CHAPTER 13. SUMMARY AND OUTLOOK

- In the presence of a magnetic superlattice (SL) on graphene we obtained collimation of an incident electron beam normal to the superlattice direction at least for large wave vectors. We showed that when using a combined magnetic and potential SL a gap can be opened with size $\Delta E = \beta |\sin P|$ that is proportional to the height of the magnetic barriers and which is a periodic function of the strength of the potential barriers. We found that in order to open a gap in such superlattices we need to have both electrical and magnetic barriers present. Furthermore, the analogy between a beam of photons and such collimated electron beams having a linear dispersion may result in novel graphene based devices which are inspired by existing opto-electronic devices.

- We found that Dirac electrons can not be confined in a circular magnetic dot due to its bent interface. Only quasi-bound states with a finite lifetime are present. The difference of those quasi-bound states between Schrödinger and Dirac electrons is mostly in the energies of these states which is a consequence of the different energies of the corresponding Landau levels. We also found that in the case of Dirac electrons a zero energy bound state exists for negative values of the angular momentum which is fundamentally different from Schrödinger electrons.

- We showed that the scattering of Dirac electrons even by azimuthal symmetric structures depends on the valley index: the $K$ valley electrons are preferentially deflected to one side (the Hall component of the resistivity isn’t zero) while the electrons of the other $K'$ valley are deflected to the other side of the sample. We proposed that this property can be used to realize a valley index filter.

Outlook

- When strain is applied to graphene it results in a pseudo magnetic field that can be used to manipulate the motion of the electrons. I expect that many of the calculations for strained graphene will be analogous to the one presented in this thesis for electron motion in nonhomogeneous magnetic field profiles. Nevertheless, one should keep in mind that there is a fundamental difference. The pseudo magnetic field does not break the time reversal symmetry. The reason is that the pseudo-magnetic field has the opposite sign in the $K$ and $K'$ valley.

- Extend the results to experimental realized magnetic field profiles which are smooth in contrast to the studied step and Dirac delta profiles.
Samenvatting van de resultaten

De volgende nieuwe resultaten en inzichten werden bekomen in deze thesis:

- Gebruikmakend van de analogie met optische stralenbundels hebben we aange- toond dat de elegante technieken uit dit domein hier aangewend kunnen wor- den, wat aanleiding geeft tot nauwkeurige resultaten voor de Dirac-vergelijking. Door de transmissie van zo’n Dirac-elektronenbundel door een enkele pn- junctie te beschouwen toonden we aan dat, ondanks dat een pn-junctie negatieve refractie toelaat voor een elektronenbundel, zoals in een optisch meta-materiaal, dit geen invloed heeft op de grootte van de minimale diameter van de elektronenbundel dewelke het essentiële kenmerk is van elke lens. Een krimpen van deze breedte is wel mogelijk als men een gebogen pn-junctie, die meer op een echte lens gelijk, gebruikt. Door het aanleggen van een periodische potentiaal samengesteld uit afwisselend pn- en np-juncties konden we aantonen dat het collimeren (gelijkrichten) van de bundel mogelijk is voor superroosters met een grote subrooster-constante en lage barrières.

- We toonden aan dat een potentiaalbarrière in grafeen, ondanks het effect van Klein-tunneling de rol van een Fabry-Pérot interferometer kan spelen. Hierbij corresponderen de potentiaalsstappen met twee parallelle spiegellende oppervlakken. Verder toonden we aan dat indien er loodrecht op het grafeen een magnetisch veld wordt aangelegd, dat de Fabry-Pérot resonanties recht- evenredig met de grootte van het magnetisch veld verschuiven.

- Door het aanleggen van een inhomogene magnetisch veld, zoals een mag- netische barrière gegenereerd door bijvoorbeeld een ferromagnetische strook, vonden we het volgende: de transmissie-waarschijnlijkheid is afhankelijk van de hoek en door de breedte van de barrière of de magnetische veldsterkte te variëren, kan men de transmissie-waarschijnlijkheid regelen. Dit toont aan
dat zulke magnetische barrières als een elektronengolf-filter gebruikt kunnen worden. Verder toonden we aan dat een superrooster van zulke barrières ons in staat stelt om een bandkloof te openen in het energie-spectrum. Deze resultaten werden uitgebreid tot twee-lagig grafeen waarbij we kwalitatief een gelijkaardig gedrag vonden.

- In de aanwezigheid van een magnetisch superrooster valt de richting van de invallende elektronenstraal samen met de richting van het superrooster, ten minste voor grote golfvectoren. We hebben aangetoond dat de combinatie van een magnetisch veld en een potentiaal SL een bandkloof kan openen waarvan de grootte $\Delta E = \beta | \sin P |$ evenredig is met de hoogte van de magnetische barrières en welke periodisch is in de sterkte van de potentiaalbarrières. We vonden dat zowel magnetische als potentiaalbarrières noodzakelijk zijn om een kloof te openen in dergelijke superroosters. Bovendien kan de analogie tussen lichtstralen en zulke gecollimeerde elektronenstralen met een lineaire dispersie resulteren in nieuwe apparaten gebaseerd op grafeen die geïnspireerd zijn door bestaande opto-elektronische toestellen.

- We vonden dat een magnetisch veld geen elektronen kan opsluiten in een cirkelvormige magnetische quantum dot. Enkel quasigebonden toestanden met een eindige levensduur zijn aanwezig. Het verschil in de quasigebonden toestanden tussen Schrödinger- en Dirac-elektronen is een gevolg van de verschillende energieën van de corresponderende Landau-toestanden. We vonden ook dat er in het geval van Dirac-elektronen gebonden toestanden met nulpuntsenergie bestaan voor negatieve impulsmomenten die fundamenteel verschillen van Schrödinger-elektronen.

- We toonden aan dat de verstrooing van Dirac-elektronen zelfs bij azimutaalsymmetrische structuren afhankt van de vallei-index: de elektronen van de K-vallei worden bij voorkeur afgebogen naar een kant (de Hall-component van de resistiviteit is niet gelijk aan nul), terwijl de elektronen van de K’-vallei naar de andere kant van het sample worden afgebogen. We stelden voor dat deze eigenschap gebruikt kan worden om een vallei-indexfilter te maken.
Bibliography


Curriculum vitae

Name: Massoud Ramezani Masir
Born: 03/09/1981, Tehran, Iran
Contact: Groenenborgerlaan 171 (U208)
         2020, Antwerpen
         Belgium
E-mail: Massoud.RamezaniMasir@ua.ac.be

Education
2008-2012: PhD in Physics, University of Antwerp, Belgium
2004-2007: Master in Physics, University of Tarbiat Modares, Iran
2000-2004: B.S. Physics, Mazandaran University, Iran

Research Interest
Electronic and transport properties of Graphene,
quantum Hall effects and topological insulator.

Computer skills
Operating systems: Windows, Linux
Office: Word, Excel, PowerPoint
Programming (basic): C/C++, Fortran
Mathematical software: MATLAB, Maple, Mathematica

Languages
Persian (native), English
Publications

Journal Articles

1. Direction-dependent tunneling through nanostructured magnetic barriers in graphene,

2. Wavevector filtering through single-layer and bilayer graphene with magnetic barrier structures,

3. Tunneling, conductance, and wavevector filtering through magnetic barriers in bilayer graphene,

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Proceedings

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- Prof. Dr. F. M. Peeters, Professor of Physics Department (Head of CMT research group), University of Antwerp, Belgium.
  Email: Francois.Peeters@ua.ac.be
- Prof. Dr. A. Matulis, Professor of Physics, Semiconductor Physics Institute, Gostauto 11, 2600 Vilnius, Lithuania.
  Email: amatulis@takas.lt
- Prof. Dr. P. Vasilopoulos, Professor of Physics, Department of Physics, Concordia University, Montreal, Quebec, Canada H3G 1M.
  Email: takis@alcor.concordia.ca