Relativistic dynamics and Dirac particles in graphene

by

Nan Gu

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Abstract

Graphene, a two-dimensional hexagonal lattice of carbon, has jumped to the forefront of condensed matter research in the past few years as a high quality two-dimensional electron system with intriguing scientific and practical applications. Both the monolayer and bilayer allotropes are of tremendous theoretical interest, each in its own specific ways.

We will focus on the transport properties of graphene in various gated configurations and magnetic fields. We proceed by stating the motivations to study these unusual materials and follow up by deriving the machinery needed to model and understand the low energy behavior. We will see that graphene offers many very strange and unexpected phenomena. We will begin with monolayer in crossed electric and magnetic fields and use the Lorentz symmetry of the Dirac equation to solve for magnetoconductance. Next, we proceed to study monolayer quasiparticles in a deconfining potential and a magnetic field. The two-dimensional nature of graphene allows us to study competition between the two external fields. Finally, a look at bilayer graphene in a p-n-p junction shows a case of confinement by chirality - where transitions between states at the same energy are forbidden by an emergent quantum property, chirality.

The purpose of this thesis is to provide a taste of the bizarre possibilities that occur in graphene, and to convince the reader that graphene really is unique and worthy of detailed study. The general writing philosophy is to use toy models to provide a simple intuitive picture, followed by a more quantitative analysis.

Thesis Supervisor: Leonid S. Levitov
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I would like to express my sincerest appreciation for the many people who have made this thesis possible. As there are so many people to thank, I will break this part down into a few pieces, starting with the people who directly contributed to the research portions of this thesis, followed by the those who have aided and guided my physics education, and last but certainly not least, those who have supported me as friends and family.

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The list can go on and on, but the thesis has to start somewhere, so I will end with this. It is rare that we have a chance to look at a segment of our lives, and reflect on those who have made an impact. From this reflection, I realize that this thesis is the product of the efforts so many people, the influences from so many different lives. So to each and every person who has impacted my life so far, I would just like to say, I like where I am, and thank you for getting me here.
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Chapter 1

Introduction

The topic of this thesis is about graphene, a two-dimensional material composed of carbon arranged in a hexagonal lattice. Graphene was first isolated and functionally discovered in 2004 [1], and in the few short years since, it has generated enormous amounts of interest in the condensed matter community. The scientific impact of a fundamentally new type of two-dimensional material was significant enough to earn its discoverers, Andre Geim and Konstantin Novoselov, the 2010 Nobel Prize in Physics. While graphene is vaunted for its potential for high quality electronic devices, which has all but ensured continuing interest and funding for years to come, this unique material also serves as a testbed for many interesting and never before observed physical effects. This thesis will focus on the intellectual curiosities that graphene has to offer, and in particular, will discuss several phenomena that can be observed in electron transport.

A second focus of this thesis is on the similar, yet vastly different carbon allotrope, bilayer graphene. The bilayer version is composed of two monolayers stacked together with carbon atoms in the two layers forming a dimerized coupling [2]. Bilayer graphene hosts as much potential for applications and curious phenomena as its single layer cousin. In Chapter 2, we\(^1\) will formulate the low energy models for monolayer and bilayer graphene, and contrast and compare the two.

In this introductory section, we will discuss the specifics of the various motivations for studying graphene systems. We assume understanding of quantum mechanics and solid

---

\(^1\)The use of “we” throughout the thesis signifies the author and the reader.
state physics at the advanced undergraduate level, but will review the most crucial concepts. As we will see, monolayer graphene provides a table top analog to ultrarelativistic electrons while bilayer graphene offers an even more unique band structure that has no high energy analog.

1.1 Comparison with the Dirac equation

The first thing most physicists will think about when they hear the word 'graphene' is the linear dispersion relation of the charge carriers. The linear spectrum, and the Hamiltonian associated with it, has a history that transcends condensed matter physics and was first proposed by P. A. M. Dirac in the search for a Lorentz invariant formulation of electron dynamics [3]. The Dirac equation also revealed the existence of antiparticles, which must be taken into account when the energies involved are much larger than the rest mass of the electron, which is always the case in graphene. We will not reproduce the basic properties of the Dirac equation here, and will refer to a graduate level textbook such as Ref. [4] for those interested.

The low energy properties of monolayer graphene are predicted to be governed by a two-dimensional massless Dirac equation [5, 6] which has been confirmed by a variety of experiments [7, 8]. Such a Hamiltonian can be written as

\[ H_{\text{MLG}} = v_F \sigma \cdot \vec{p} = v_F \begin{pmatrix} 0 & p_x - i p_y \\ p_x + i p_y & 0 \end{pmatrix}, \quad \epsilon(\vec{p}) = \pm v_F |\vec{p}|, \quad (1.1) \]

where \( v_F \approx 10^8 \text{ cm/s} \) is the Fermi velocity, the \( \pm \) sign refers to the conduction band (positive energy states) and valence band (negative energy states), respectively. The quantity \( \sigma \) denotes pseudospin, an analog of true spin that exists because of the hexagonal symmetry of the graphene lattice. We will go through a derivation of this Hamiltonian and go into more detail on the origin of pseudospin in Section 2.1.2. As we see in the structure of Eq. 1.1, and as we will show in Section 2.1.2, the pseudospin is correlated with the direction of propagation.

The analog between the normal treatment of the Dirac equation and the governing
Hamiltonian for monolayer graphene is virtually perfect, save for three distinctions. One difference refers to the two-dimensional nature of graphene, which only necessitates a two component spinor, as opposed to the 4 components in the 3D case. The second difference is the massless nature of the graphene dispersion relation, which essentially puts graphene in the ultrarelativistic limit of the Dirac equation, when the mass becomes negligible. The final difference is the velocity factor multiplying the momentum is the Fermi velocity $v_F$ instead of the speed of light $c = 3 \times 10^{10}$ m/s. Keeping these three facts in mind, we see that, graphene provides a way to access the physics of Dirac electrons, and this correspondence opens up many possibilities to test high energy physics on a tabletop setup. We will describe a few of the peculiarities of Dirac electrons in the next subsections.

### 1.1.1 Klein tunneling

Perhaps the most striking transport prediction for Dirac electrons is Klein tunneling in the ultrarelativistic limit [9]. Imagine a system where a massless Dirac particle of energy $\epsilon$ is in a monotonic potential, which only depends on $x$, that satisfies $U(x \to -\infty) = U_1$, $U(x \to \infty) = U_2$, where $U_1 < \epsilon < U_2$. In such a configuration, a normally incident electron from the left will transmit through the potential with 100% probability, independent of $\epsilon$. There are two key elements here that guarantee perfect transmission; one is the fact that massless Dirac electrons have a dispersion relation that allows states to exist continuously from the positive energy continuum down to the negative energy continuum. Two is a subtle effect of chirality, where states propagating in one direction maintain the same chirality. Therefore, in the absence of chirality changing interactions, backscattering at normal incidence in p-n junctions is forbidden.

However, to realize Klein tunneling in real electrons, we must create an enormous electric field, so that we may overcome the mass gap, and access the negative energy states. Such a field would require an energy difference of $2m_e c^2$ generated over a distance of a Compton wavelength $\hbar/m_e c$, as calculated by Sauter [10]. The field required in free space is in excess of $10^{16}$ V/cm. Graphene, however, offers a more feasible alternative, requiring no minimum field, since its quasiparticles are massless. Studies on Klein tun-
neling in graphene have predicted virtually the same phenomena as its high energy counterpart [11, 12, 13]. We will explore Klein tunneling in monolayer graphene as well as its analog in bilayer graphene in more detail in Chapter 2. In Chapters 3 and 5, we will construct explicit systems where the effects of this type of tunneling can be measured.

Understanding Klein tunneling will also help elucidate the topic of minimal conductivity in monolayer graphene [7, 14, 15, 16, 17, 18], a topic that we will not cover in this thesis, but is very interesting and still under debate.

1.1.2 Lorentz invariance

Another quality that distinguishes the Dirac equation from the Schrödinger equation is Lorentz invariance. Since the development of Special Relativity in the early 20th century, we have known that Galilean invariance is not a true symmetry of spacetime, but instead reference frames are actually linked by Lorentz transformations. In graphene, we can use a modified version of this symmetry to simplify a system involving electric and magnetic fields, as Maxwell’s equations also respect Lorentz symmetry [19]. We must be mindful that the velocity for graphene is $v_F$ rather than $c$, so that the scale factor for time is different. As we will see in Chapter 3, one can perform a boost and transform away either the electric field or the magnetic field [20, 21]. The system is more easily solved in this frame, and boosting back to the “lab” frame yields the observable result. As a result, we can bring the formalism and intuition developed for Special Relativity to use in graphene.

1.2 Berry phase

In 1983, Michael Berry discovered that, given a Hamiltonian $H(\vec{R})$ that depends on some parameters $\vec{R} = \{X, Y, \ldots\}$, a quantum state taken adiabatically along a closed path in parameter space will acquire a nontrivial phase factor [22]. We can show that this phase has physical significance by considering an interference experiment between a state that remains at $\vec{R}$ and one that acquires a phase by evolving around a closed path (in time $T$) such that $\vec{R}(t = 0) = \vec{R}(t = T)$. The states will interfere constructively or destructively based on the phase accumulated. This phase, called a Berry phase, only depends on the path traveled.
in parameter space and not the rate of evolution, in contrast to the more familiar dynamical phase. Formally, if we have a set of eigenstates that obey $H(\vec{R})|n(\vec{R})\rangle = E_n(\vec{R})|n(\vec{R})\rangle$ for any given $\vec{R}$, then the adiabatic time evolution of a state $|n(\vec{R}(t = 0))\rangle$ from time 0 to time $t$ is given by

$$|\psi(t)\rangle = \exp\left[\frac{i}{\hbar} \int_0^t dt' E_n(\vec{R}(t')) \right] e^{i\gamma_{n}(t)}|n(\vec{R}(t))\rangle. \tag{1.2}$$

Inserting this wavefunction into the Schrödinger Equation, $i\hbar|\psi(t)\rangle = H(\vec{R}(t))|\psi(t)\rangle$, we find that the Berry phase can be written as:

$$\gamma_n(C) = i \oint_C \langle n(\vec{R})|\vec{\nabla}_{\vec{R}}|n(\vec{R})\rangle \cdot d\vec{R}, \tag{1.3}$$

where $C$ is a the closed path in parameter space that we have evolved along and $\vec{\nabla}_{\vec{R}}$ is the vector derivative with respect to $\vec{R}$.

The simplest system in which to study the Berry phase is an electron in a constant magnetic field that slowly changes direction. The Hamiltonian and eigenstates for this system are

$$H(\vec{B}) = \frac{\hbar e B}{2m_e} \vec{\sigma} \cdot \vec{B}, \quad \chi_+ = \begin{pmatrix} \cos(\theta/2) \\ e^{i\phi} \sin(\theta/2) \end{pmatrix}, \quad \chi_- = \begin{pmatrix} \sin(\theta/2) \\ -e^{i\phi} \cos(\theta/2) \end{pmatrix}, \tag{1.4}$$

where $\theta$ and $\phi$ are the polar and azimuthal angles, as defined by $\vec{B} = B \sin \theta \cos \phi \ \hat{x} + B \sin \theta \sin \phi \ \hat{y} + B \cos \theta \ \hat{z}$. Now the gradient with respect to $\vec{B}$ simply the gradient in spherical coordinates with a constant magnitude, $1/B$. Evaluating the Berry phase given by Eq. 1.3 with the states in Eq. 1.4, we find $\gamma_\pm = \mp \Omega/2$, where $\Omega$ is the solid angle swept out by the closed path on a sphere.

The relationship to monolayer graphene can realized by observing that the Dirac Hamiltonian is of the exact form of the Hamiltonian in Eq. 1.4, with the magnetic field $\vec{B}$ replaced by the momentum $\vec{p}$ (up to scale factors). However, since $\vec{p}$ is restricted to live in a two-dimensional plane, the only closed loops that can form enclose $2\pi$ steradians, yielding a Berry phase of $\gamma = \pi$. This additional phase factor exists when the momentum winds
around the Dirac cone, and thus requires electrons to move in a circle.

A realization of this effect can be achieved in the Quantum Hall regime, where the additional $\pi$ Berry phase gives rise to what is known as the anomalous Quantum Hall effect [23, 24, 7]. A second realization can be done in by setting up a monolayer graphene p-n-p junction [25]. The conductance displays resonances analogous to Fabry-Pérot resonances, where the two p-n junctions act as etalons. If a sufficiently strong magnetic field is introduced, the trajectories can curve enough within the central n region so that a full rotation of the particle is achieved. When this occurs, an additional Berry phase of $\pi$ is included in the Fabry-Pérot calculation, yielding a half period phase shift of the resonances.

The low energy Hamiltonian for bilayer graphene also contains a Berry phase for closed orbits. We can write the bilayer Hamiltonian as [2]

$$H_{\text{BLG}}^{\text{BLG}} = \frac{1}{2m} \begin{pmatrix}
0 & (p_x - ip_y)^2 \\
(p_x + ip_y)^2 & 0
\end{pmatrix} = \epsilon(p) \vec{\sigma} \cdot \hat{n}, \quad \epsilon(p) = \frac{p_x^2 + p_y^2}{2m},$$

(1.5)

where $m \approx 0.04m_e$ is the band mass for bilayer electrons and the two components denote wavefunction amplitudes on the $B_1$ and $A_2$ sites (see Section 2.1.3). The unit vector $\hat{n} = (\cos 2\theta, \sin 2\theta)$ is parameterize using the angle $\theta$ defined by $\hat{p} = (\cos \theta, \sin \theta)$. Thus we see the bilayer Hamiltonian also fits the form of Eq. 1.4, except, instead of $\pi$, a Berry phase of $2\pi$ is enclosed [26, 2] when a particle traces out a closed path. A phase of $2\pi$ cannot have a physical effect in the classical limit, but can have effects in the quantum limit. In particular, in the Quantum Hall effect, there is an additional degenerate state at zero energy due to this Berry phase [26, 2]. Recently, it has been suggested that the $2\pi$ Berry phase for bilayer graphene can be interpreted as 0 Berry phase plus a winding number [27].

### 1.3 Structural properties and use of external fields

There are practical considerations that make both monolayer and bilayer graphene very attractive for theoretical and experimental reasons. We will go over the main reasons in this section.
1.3.1 Simplicity and purity

Perhaps the most compelling experimental reason to work with graphene is the ease of creating a sample. While similar two dimensional electron gas systems exist, such as GaAs quantum wells, they are difficult and expensive to create. Graphene, on the other hand, can be made using a good graphite sample and a few tools [1]. The simplicity of creating a good graphene sample has allowed the field the proliferate greatly, and along with improvements in fabrication techniques, many theoretical predictions can be tested in just a few short months.

Graphene is also attractive theoretically because it is very clean, which allows us to model the system using simple single particle quantum mechanics. The strong carbon-carbon bonds that make up the hexagonal graphene lattice suppresses defects. As a result, monolayer and bilayer graphene samples have fairly high mobilities, ~ 15,000 cm²/Vs on SiO$_2$ [28], > 20,000 cm²/Vs on hexagonal boron nitride [29], and up to ~ 200,000 cm²/Vs with a suspended sample [30, 31]. Such high mobilities, indicative of a long mean free path, which can reach order μm [30], allows for the probing of ballistic effects, such as Klein tunneling, or the Berry phase as mentioned in Sections 1.1.1 and 1.2. We should note, however, that many applications require depositing dielectrics and local gates on the samples, lowering their mean free paths to sub-100 nm scales [10]. Therefore, any attempt to manipulate those samples lowers their quality, which is addressed in the following section.

1.3.2 Field effect

The carrier density of many materials can be tuned using the field effect [1, 7], where a gate is placed some distance away from the sample, separated by a dielectric. Altering the voltage on the gate allows for charging/depleting carrier density, just like a parallel plate capacitor. Graphene is special because it is a true freestanding two-dimensional material, where the electrons are fully accessible to the outside. The distance between the gate and the sample is just determined by the thickness of the dielectric coating and can be as small as ~ 5 nm [10]. The distance to the gate sets the length scale of the potential variations in the sample, and as a result, we can create junctions and junction combinations that vary
on a scale much smaller than the mean free path to explore ballistic effects in various configurations [32]. We will indeed find that this property is crucial for probing the results in Chapters 3, 4, and 5 when we consider ballistic effects.

1.3.3 Bilayer graphene - tunable band gap

Perhaps one of the greatest hurdles of using graphene as a semiconductor substitute is the lack of a band gap. The band gap in semiconductors is used to create a large on/off current ratios in devices, such as transistors. The problem is only exacerbated by the minimal conductivity of graphene, which allows current to flow at the Dirac point, where the density of states vanishes. Although there are many proposals to create a band gap in monolayer graphene, such as with nanoribbons [33, 34], or epitaxial graphene grown on SiC [35], or subjecting graphene to a superlattice that breaks inversion symmetry [36], each has severe limitations.

This is where bilayer graphene comes to the rescue. Since the two components of the low energy Hamiltonian of bilayer graphene originate on different layers (see Section 2.1.3), we can in fact open a gap by applying a transverse electric field [37, 38, 39, 40, 41]. Not only does this alleviate the problem of not having a band gap, a tunable gap is very interesting because we introduce an additional tunable parameter into our Hamiltonian, allowing us to change the pseudospin and alter transport properties. For example, the bilayer graphene Hamiltonian (Eq. 1.5) $H^{BLG} \sim \vec{\sigma} \cdot \vec{n}$ possesses a quantum number closely related to chirality, as we see that the pseudospin is correlated with the direction of propagation. Now if we add a gap, we will alter that correlation. As we will derive in Section 2.3 and Chapter 5, the addition of a gap changes transport properties significantly.

1.4 Organization of this thesis

From the interesting structure of the Hamiltonians, to the various control parameters available, we have aptly described our motivation for studying graphene. Now we move on to a short summary of the chapters to come.
1.4.1 Models and methods

In this chapter, we will build up the models and methods needed to understand the effects in Chapters 3, 4, and 5. We will begin with the structure of graphene and eliminate degrees of freedom until the low energy Hamiltonians for monolayer and bilayer have been obtained. We will also compare and contrast the two materials, particularly in their chiral characteristics. Finally, we will formalize the connection between models and experimental observables.

1.4.2 Zener-tunneling and magneto-resistance in p-n junctions

We begin our analysis of graphene transport in the simplest gated geometry available, monolayer graphene in a single p-n junction. Through a simple substitution, we will show that the transmission amplitude can be mapped directly onto the tunneling amplitude in the Landau-Zener problem, and that this solution is consistent with the heuristics of Klein tunneling. Motivated by the similarity of the monolayer graphene Hamiltonian to the Dirac Hamiltonian, we will use the Lorentz invariant structure (with \( v_F \) acting as the speed of light) to study the behavior of transmission in weak magnetic fields. Specifically, we will boost (using the drift velocity) to a frame where the magnetic field vanishes, apply the \( B = 0 \) solution, and boost back to the lab frame. Finally, we will derive a measurable effect in form of magneto-resistance.

1.4.3 Landau level collapse in gated graphene

The next system we study is locally gated monolayer graphene gated in a p-p′-p configuration with a uniform magnetic field. We analyze the competition between the localizing effects of a strong magnetic field and the delocalizing tendencies of a repulsive electrostatic potential. In a high magnetic field, Landau levels persist and the spectrum is quantized, whereas in the low magnetic field limit, a continuum of extended states exist. This phenomenon is not inherent to graphene alone, but was not observed until now due to the difficulties in gating a traditional 2D electron system on a scale comparable to the magnetic length. We predict the dependence of the critical magnetic field on potential shape and
strength and offer a semiclassical description using electron orbits.

1.4.4 Chirality-assisted confinement in bilayer p-n-p junctions

Finally, we move onto bilayer graphene and the so-called anti-Klein tunneling effect. In a p-n-p junction, we describe the presence of bound states that are completely decoupled from the continuum outside at normal incidence. The decoupling stems purely from the opposite chiralities of quasiparticles and quasiholes. We set up a model to approximate particle transmission profiles and use this to compute the ballistic conductance, which shows a distinctive shape due to the decoupled states. Since real bilayer graphene devices often have an interlayer bias at finite carrier densities, we also discuss the effects of a gap.
Chapter 2

Models and methods

2.1 Electronic properties of graphene

In this section we introduce the crystalline structure of graphene as well as the models necessary to describes its electronic behavior at low energies. We will briefly mention the chemical basis for using the tight-binding model and continue on to the continuum model. We then use the continuum model for single layer graphene, along with the structure of bilayer graphene to derive a low energy continuum Hamiltonian for bilayers.

2.1.1 Tight-binding model

Graphene is a two dimensional hexagonal lattice of carbon atoms, literally one atom thick. Of the four $n = 2$ atomic orbitals of carbon, $s$, $p_x$, and $p_y$ hybridize into three $sp^2$ orbitals, angled $120^\circ$ apart from each other in the $x$-$y$ plane. The $sp^2$ orbitals on adjacent carbon atoms form $\sigma$-bonds, the strongest form of covalent bonds. The $\sigma$-bonds lock the carbon into a hexagonal lattice, giving graphene its characteristic structure. As a result, the low energy physical model only involves the remaining $p_z$ orbitals, which form much weaker $\pi$-bonds. From this perspective, we begin with the tight-binding approximation assuming $p_z$ orbitals with small overlap.

The Bravais lattice of graphene contains two carbon atoms per units cell, as a result, the tight-binding Hamiltonian can be written as a $2 \times 2$ matrix. In the simplest approximation,
Figure 2-1: (a) Band structure for graphene, showing the valence and conductance bands touching at the Dirac points. The dispersion around the Dirac points are approximately linear. (b) Momentum space plot of the valence band (minus sign in Eq. 2.2) showing contours of constant energy. Note that the contours surrounding the Dirac points are approximately circular, yielding an isotropic dispersion relation near those points.

we only take into account nearest neighbor interactions, and the Hamiltonian can be written as

\[ H_{\text{TB}}^{\text{MLG}} = \begin{pmatrix} 0 & \tau(k) \\ \tau^*(k) & 0 \end{pmatrix}, \quad \tau(k) = \sum_i t e^{i\vec{\mu}_i \cdot \vec{a}_i}, \tag{2.1} \]

where \( \vec{\mu}_i \) are the nearest neighbor lattice vectors with \( i = 1, 2, 3 \). The interatomic spacing is \( a = 2.46 \) Å and the tight-binding hopping parameter is \( t \approx 3 \) eV. We have suppressed the on diagonal component of the energy, since it is just a constant in the nearest neighbor approximation. For definiteness, we choose our nearest neighbors such that \( \vec{\mu}_1 = a\hat{x}, \vec{\mu}_2 = -\frac{1}{2}a\hat{x} + \frac{\sqrt{3}}{2}a\hat{y}, \) and \( \vec{\mu}_3 = -\frac{1}{2}a\hat{x} - \frac{\sqrt{3}}{2}a\hat{y} \). Now, solving for the energies of the Hamiltonian (Eq. 2.1) yields

\[ E(\vec{k}) = \pm t \left| e^{i\vec{k}\cdot\vec{a}} + e^{-i\vec{k}\cdot\vec{a}/2} \left( e^{i\sqrt{3}/2k_y a} + e^{-i\sqrt{3}/2k_y a} \right) \right|, \tag{2.2} \]

where \( \pm \) denote the conduction and valence bands, respectively.

The resulting band structure shows that the valence and conduction bands touch at points known as Dirac points. At the Dirac points, the dispersion is approximately linear and isotropic, reminiscent of ultrarelativistic Dirac electrons. Note that there are only two
inequivalent Dirac points in the first Brillouin zone, since the other points can be related by translation of a reciprocal lattice vector. Since carbon has one electron per \( p_z \) orbital, at zero doping, the lower band must be completely filled, while the upper band is completely empty. Hence, to explore the low energy dynamics we can expand the Hamiltonian (Eq. 2.1) near the Dirac points.

### 2.1.2 Continuum model - Dirac equation

Following along with the philosophy that we wish to model only the low energy behavior of electrons in graphene, we can expand the Hamiltonian (Eq. 2.1) around the Dirac points. Again, for definitiveness, we will choose our two inequivalent Dirac points as \( \pm \vec{K} = \pm \frac{4\pi}{3\sqrt{3}a} \hat{\gamma} \). To first order in \( \vec{k} \), the expansion gives:

\[
H_{\pm \vec{K}}^{\text{MLG}} = \hbar v_F \begin{pmatrix}
0 & ik_x - ik_y \\
-ik_x + ik_y & 0
\end{pmatrix},
\tag{2.3}
\]

where the low energy wavefunction takes the form of:

\[
\Psi(\vec{r}) = \begin{pmatrix}
u_{\vec{K}}(\vec{r}) \\
v_{-\vec{K}}(\vec{r})
\end{pmatrix} e^{i\vec{K} \cdot \vec{r}} + \begin{pmatrix}
u_{-\vec{K}}(\vec{r}) \\
u_{\vec{K}}(\vec{r})
\end{pmatrix} e^{-i\vec{K} \cdot \vec{r}}.
\tag{2.4}
\]

where \( u_{\pm \vec{K}}(\vec{r}) \) and \( v_{\pm \vec{K}}(\vec{r}) \) are slowly varying envelope functions of the more rapidly oscillating \( e^{\pm i\vec{K} \cdot \vec{r}} \) terms. We note that the wavevectors \( \pm \vec{K} \) can only be coupled to each other by a potential that varies on the scale of \( a \), the lattice spacing. In the absence of lattice scale scatterers, the two \( \pm \vec{K} \) points can be treated essentially independently. For effects that do not depend on lattice orientation, we can simply solve the Hamiltonian (Eq. 2.3) for one Dirac point, and multiply by a degeneracy factor of 2. Keeping this simplification in mind, we will work with only the \( + \vec{K} \) Dirac point. If we rotate the Pauli matrices in Eq. 2.4 accordingly, we obtain the Dirac equation form of the monolayer graphene Hamiltonian (Eq. 1.1).

We should pause here to make a few notes. First, since there are two identical carbon atoms in each unit cell, the relative weight of the wavefunction on each atom gives rise to
an $SU(2)$ spin structure. For each electron, the amplitudes on the A and B sites determine the pseudospin. Second, the range of validity of this Dirac Hamiltonian is sufficiently broad for most transport purposes. In the low energy limit, the exact symmetry between the two sublattices is broken by the spin-orbit interaction, yielding a very small gap of order 1 $\mu$eV [42, 43]. Another way to generate a gap is through the Rashba interaction with an electric field perpendicular to the sample. Such fields can be created by the gates that control carrier density or by impurities in the substrate. Estimates of this gap for large gate voltages are also on the order of 1 $\mu$eV [42]. At higher energies, the isotropic linear approximation to the band structure breaks down at $\sim 500$ meV. The energy range of validity for the Dirac Hamiltonian (up to 500 meV) offers a very broad range of carrier densities ($n$ up to $10^{13}/cm^2$) to explore, with experiments typically using densities of $n \sim 10^{12}/cm^2$ [32].

2.1.3 Bilayer continuum model

We now move on to establish the model Hamiltonian we will use for bilayer graphene. Instead of building up from a tight binding perspective, we will instead view bilayer graphene as two stacked monolayer sheets on top of each other as shown in Figure 2-2. The stacking is such that the atoms of the $A_1$ sublattice are directly on top of the atoms of the $B_2$ sublattice, where the subscript denotes the layer index. The $B_1$ and $A_2$ atoms are positioned over the centers of the hexagons of the other layer. By using the Dirac Hamiltonian for each monolayer, and including the coupling between the $A_1$ and $B_2$ atoms, the resulting $4 \times 4$ Hamiltonian can be written in the $\{A_1, B_1, A_2, B_2\}$ basis as

$$H^{BLG}_{4\times4} = \begin{pmatrix}
\Delta & v_F p_- & 0 & \gamma_1 \\
v_F p_+ & \Delta & 0 & 0 \\
0 & 0 & -\Delta & v_F p_- \\
\gamma_1 & 0 & v_F p_+ & -\Delta
\end{pmatrix}, \quad (2.5)$$

where $p_\pm = p_x \pm ip_y$, the interlayer coupling $\gamma_1 \approx 0.4$ eV [2], and where we have allowed for the possibility of an interlayer bias, $\Delta$. At $p_x = p_y = 0$ and $\Delta = 0$, we clearly see that
the four resulting bands include two at energy $\epsilon = 0$ and two at $\epsilon = \pm \gamma_1$. We can then treat the interlayer coupling as a large parameter and following Ref. [2], we can reduce the Hamiltonian to a two band model written as

$$H_{BLG} = \begin{pmatrix} \Delta & \frac{p^2}{2m} \\ \frac{p^2}{2m} & -\Delta \end{pmatrix}, \quad (2.6)$$

where $m = \frac{\gamma_1}{2\sqrt{3}}$. The two components of the spinor now correspond to the $\{B_1, A_2\}$ atomic sites, and the dimerized $A_1-B_2$ atoms have been integrated out. The energy bands of this Hamiltonian are $\epsilon(\vec{p}) = \pm \sqrt{\left(\frac{p^2}{2m}\right)^2 + \Delta^2}$, where $p^2 = p_x^2 + p_y^2$. We will use this two band model throughout this thesis.

We should also discuss the limits of validity for the two band model of bilayer graphene. At high energies, this model is valid as long as the two higher bands are not occupied. This restriction limits the allowed energies to be $\epsilon < \frac{1}{4} \gamma_1 \approx 100$ meV [2]. In the $\epsilon \to 0$ limit, a "trigonal warping" term that is not included in Eq. 2.6 dominates the dispersion relation below $\epsilon \approx 5$ meV. In terms of carrier density, and assuming the gap $\Delta \ll \epsilon$, we find the range of validity to be $n \sim 10^{11} / \text{cm}^2$ to $10^{12} / \text{cm}^2$.

### 2.2 Chirality in single layer graphene

Chirality in single layer graphene manifests identically to chirality in the ultrarelativistic Dirac equation. There are two eigenvalues of the chirality operator, $(\vec{\sigma} \cdot \vec{p})\psi_{\pm} = \pm \psi_{\pm}$, which
The relationship between pseudospin and momentum in monolayer graphene. The pseudospin points parallel (antiparallel) to the momentum in the conduction (valence) band. The velocity is also shown. b) The same relationship in bilayer graphene. For a rotation of angle $\theta$ the momentum $\vec{p}$, the pseudospin rotates $2\theta$. For a fixed momentum, the pseudospin in the conduction and valence bands point in opposite directions.

2.2.1 Klein tunneling

We begin with the Dirac Hamiltonian for monolayer graphene (Eq. 1.1) in a potential $V(x)$ that only varies in the $x$-direction,}

$$H = \nu_F \vec{p} \cdot \vec{\sigma} + V(x) = \begin{pmatrix} V(x) & \nu_F(p_x - ip_y) \\ \nu_F(p_x + ip_y) & V(x) \end{pmatrix}. \quad (2.7)$$

Since the potential is translation invariant in the $y$-direction, $p_y$ is conserved. For simplicity, we will choose $V(x)$ to be a step function, so that the wavefunctions on each side of the junction are simply plane waves. The potential can be written as

$$V(x) = \begin{cases} -V_0/2 & x < 0 \\ V_0/2 & 0 < x \end{cases}, \quad \Psi(x,y) = \begin{pmatrix} a \\ b \end{pmatrix} e^{ik_xx + ik_yy}. \quad (2.8)$$
For particular wavenumbers, we define \( (k_x \pm ik_y)/|k| = e^{\pm i\theta} \), where \( |k| = \sqrt{k_x^2 + k_y^2} \). Note that if \( k_x \) or \( k_y \) changes, the phase \( e^{i\theta} \) must change accordingly as well. Using this notation, we find the eigenvalues and wavefunctions to be

\[
E = V(x) \pm v_F|\vec{p}|, \quad \Psi_\pm(x, y) = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm e^{-i\theta} \\ 1 \end{pmatrix} e^{ik_xx+ik_yy}, \tag{2.9}
\]

where \( \vec{p} = \hbar \vec{k} \). Now let us consider the situation when we have an incident plane wave of energy \( E = 0 \) on the left. For \( x < 0 \), we must take the plus sign in Eq. 2.9 to satisfy the energy relation, whereas for \( x > 0 \), we must take the minus sign. Another constraint we must satisfy is the conservation of flux, which can be enforced by inspecting the velocity in the \( x \)-direction, \( v_x = \partial_{p_x} E(\vec{p}) = \pm v_F p_x/|\vec{p}| \). Since the + sign corresponds to the conduction band and the − sign to valence band, if the \( x \)-momentum of the particle is \( p_x \) left of the junction then it must be \(-p_x \) right of the junction. Thus, we can write the wavefunctions for \( x < 0 \) and \( x > 0 \) as

\[
\Psi_\leq = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\theta} \\ 1 \end{pmatrix} e^{ik_xx+ik_yy} + \frac{r}{\sqrt{2}} \begin{pmatrix} -e^{i\theta} \\ 1 \end{pmatrix} e^{-ik_xx+ik_yy}, \quad \Psi_\geq = \frac{t}{\sqrt{2}} \begin{pmatrix} e^{i\theta} \\ 1 \end{pmatrix} e^{-ik_xx+ik_yy}. \tag{2.10}
\]

Note that the phases of the pseudospinors change depending on the direction of propagation. Requiring continuity at \( x = 0 \) yields the equations

\[
e^{-i\theta} - re^{i\theta} = te^{i\theta}, \tag{2.11}
\]

\[
1 + r = t, \tag{2.12}
\]

which can be solved for the transmission and reflection probabilities \(|t|^2 = \cos^2 \theta \) and \(|r|^2 = \sin^2 \theta \), respectively.

When the incident particle is normal to the barrier, \( p_y = 0 \), so that \( \theta = 0 \), we find the transmission probability \(|t|^2 \) to be unity. The unitary transmission at normal incidence, independent of the strength of \( V_0 \), is the essence of Klein tunneling. A heuristic way to understand this transmission profile is to look at the pseudospin overlap between incident and
transmitted wavefunctions in Eq. 2.10, which simply yields $|\langle \Psi_{\text{inc}} | \Psi_{\text{trans}} \rangle|^2 \sim \cos^2 \theta$. This relationship is depicted in Figure 2-4. With this insight, we can understand that Klein tunneling is due to pseudospin matching between the conduction and valence bands. Although frequently called a paradox, the physical picture of Klein tunneling is clear from having an available state in the valence band, and enforcing pseudospin conservation. Finally, we should remind ourselves that even though the potential $V(x)$ was a step function, we have worked under the assumption that the potential is smooth on the lattice scale, so as to avoid scattering between the $\vec{k}$ and $\vec{k}'$ points.

2.3 Chirality in bilayer graphene

Electrons in bilayer graphene are not chiral in same sense as relativistic electrons. Instead, the quasiparticles are described by Eq. 1.5. Simply put, the pseudospin rotates twice as fast as the momentum, as shown in Figure 2-3b). This relationship between pseudospin and momentum gives rise to an effect which can be described as the “opposite” of Klein tunneling, as shown below.
2.3.1 Anti-Klein tunneling

For the analog of Klein tunneling in bilayer graphene, we begin analogously with the monolayer case, with the two band Hamiltonian (Eq. 2.6) in a potential $V(x)$ that only varies in the $x$-direction,

$$H = \begin{pmatrix} V(x) & (\frac{p_x - ip_y}{2m})^2 \\ (\frac{p_x + ip_y}{2m})^2 & V(x) \end{pmatrix}. \quad (2.13)$$

Again, $p_y$ is conserved and for simplicity, we will choose $V(x)$ to be a step function, as in Eq. 2.8. Using the same notation as in Section 2.2.1 the energies and eigenstates are

$$E = V(x) \pm \frac{p_x^2 + p_y^2}{2m}, \quad \Psi_{\pm}(x, y) = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm e^{-2i\theta} \\ 1 \end{pmatrix} e^{i k_x x + i k_y y}. \quad (2.14)$$

Using the same approach as in Section 2.2.1, let us consider the situation of an incident plane wave of energy $E = 0$ to the left of the junction. For $x < 0$, we take the plus sign in Eq. 2.14 and for $x > 0$, we take the minus sign. The quasiparticle velocity is $v_x = \partial_{p_x} E(\vec{p}) = \pm p_x / 2m$, so similar to the Klein tunneling case, if we have $x$-momentum $p_x$ to the left of the junction then the $x$-momentum must be $-p_x$ to the right. Finally, the wavefunctions on both sides of the junction are

$$\Psi_< = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-2i\theta} \\ 1 \end{pmatrix} e^{i k_x x + i k_y y} + \frac{r}{\sqrt{2}} \begin{pmatrix} e^{2i\theta} \\ 1 \end{pmatrix} e^{-i k_x x + i k_y y}, \quad \Psi_> = \frac{t}{\sqrt{2}} \begin{pmatrix} -e^{2i\theta} \\ 1 \end{pmatrix} e^{-i k_x x + i k_y y}. \quad (2.15)$$

Requiring continuity at $x = 0$ yields the equations

$$e^{-2i\theta} + re^{2i\theta} = -te^{2i\theta}, \quad (2.16)$$

$$1 + r = t. \quad (2.17)$$

Solving these equations gives the transmission and reflection probabilities $|t|^2 = \sin^2(2\theta)$ and $|r|^2 = \cos^2(2\theta)$, respectively. From these equations, we see that when the incident particle is normal to the interface, $p_y = 0$, $\theta = 0$, and no transmission may occur, despite the presence of states at the same energy on the other side of the junction. With this un-
Figure 2-5: A picture of anti-Klein tunneling with the incident particle in solid green, the transmitted particle in solid blue, and the reflected particle in dotted green. In bilayer graphene, we can see that the incident and reflected states have the same pseudospin, while the transmitted state has the opposite pseudospin. Thus, full reflection is provided by pseudospin conservation.

understanding, we can see why this phenomenon may be called “anti-Klein tunneling”, as it completely suppresses the coupling between the positive and negative energy states. Much like in the Klein tunneling case, we can understand the lack of coupling by taking the pseudospin overlap between incident and transmitted states in Eq. 2.15. Figure 2-5 shows the pseudospin orientation of the incoming, transmitted, and reflected states. The result $|\langle \Psi_{\text{inc}} | \Psi_{\text{trans}} \rangle|^2 \sim \sin^2(2\theta)$ shows the orthogonality of the incident and transmitted states at normal incidence.

It is worth to note that although this toy model predicts unitary transmission at certain oblique angles, this property is guaranteed for a more general potential. However, there is also work indicating that the addition of gap of a certain size can restore Klein tunneling [44].

We should note here that anti-Klein tunneling suppresses the coupling between plane waves on the two sides of the junction, but plane waves on one side of the junction may still couple to evanescent states on the other side. Assuming a junction of finite size, the dispersion of bilayer graphene allows for states with imaginary $x$-momenta to satisfy the energy relation in Eq. 2.14. This effect is just the normal quantum tunneling that we are familiar with. Since there are two tunneling mechanisms, which may interfere, in general, we should expect a Fano resonance instead of a Breit-Wigner peak. We will touch on this topic in Chapter 5.
2.4 Relation to transport - conductance

Now that we have the model Hamiltonians for monolayer and bilayer graphene, we need to derive quantities that are measurable in an experimental apparatus. In particular, we will use conductance as our observable. In this section, first we derive conductance using a general transmission picture, and then we show that in weak magnetic fields, the conductance will oscillate for quantized momentum orbits.

2.4.1 Landauer formula

Throughout this thesis, we will explore phenomena in graphene under the influence of external fields. However, we will restrict ourselves to fields that only break translational invariance in one direction, say $x$. As a result, we can treat our system like a series of one-dimensional systems, parameterized by the conserved momentum $p_y$.

The Landauer formalism [45, 46, 47] allows us to view a one-dimensional conductance problem as a transmission problem instead. Imagine a two-terminal system where electrons thermalize in the leads, but are phase coherent in the sample. We will assume that all of the channels in a single lead are decoupled, as is the case in graphene, since a state with conserved momentum $p_y$ can only couple to another state with the same momentum $p_y$. The electric current from a single channel $n$, from one of the leads $\pm$, at a particular energy $E$ is given by

$$I_{\pm,n,E} = \pm g e t_n^*(E) t_n(E) v(E),$$

(2.18)

where $g$ is the degeneracy, $t_n(E)$ is the transmission amplitude in the $n$ channel, and $v(E) = dE/d(\hbar k)$ is the velocity. The net current is then just the sum over all channels, leads, and energies of $I_{\pm,n,E}$ weighted by the occupation number i.e. the Fermi function

$$I = \frac{g e}{2 \pi \hbar} \sum_n \int_0^\infty dE \left[ f(E - \mu_+) - f(E - \mu_-) \right] T_n(E),$$

(2.19)

where we have used the transmission probability $T_n(E) = t_n^*(E) t_n(E)$. This integral can be evaluated very simply in the limit of zero temperature and small chemical potential.
differences in the leads \(|\mu_+ - \mu_-| \ll \mu_+, \mu_-\)

\[
I = \frac{ge}{\hbar} \sum_n T_n(E)(\mu_+ - \mu_-).
\] (2.20)

If the chemical potential imbalance is due to a voltage difference \(\mu_\pm = eV_\pm\), then we can extract the conductance from this formula as:

\[
G = \frac{ge^2}{\hbar} \sum_n T_n(E).
\] (2.21)

This simple formula is known as the Landauer formula for conductivity. We will be using this formula frequently to calculate conductance from our models.

2.4.2 Density of states and Shubnikov-de Haas oscillations

Another method we will use to relate our results to experiments involves linking oscillations in the density of states with conductance oscillations in a magnetic field. Following an argument due to Onsager [48], we can use the Bohr-Sommerfeld quantization condition on the canonical momentum as well as the semiclassical equations of motion for the kinetic momentum to derive the flux quantization

\[
\oint \left( \vec{p} + \frac{q}{c} \vec{A} \right) \cdot d\vec{r} = (n + \gamma)\hbar = \frac{q}{c} BA_r,
\] (2.22)

where \(A_r\) is the area of the sample in real space, and \(\gamma\) is a zero-point offset that is irrelevant for our semiclassical discussion. We also know that in the semiclassical approximation, the \(\vec{k}\) space orbit area \(A_k\) can be related to \(A_r\) by \(A_r = \ell_B^2 A_k\), where \(\ell_B = \sqrt{\hbar eB}/c\) is the magnetic length. Putting all this together, we arrive at a condition for the \(\vec{k}\)-space orbit

\[
A_k = \frac{2\pi eB}{\hbar c} (n + \gamma).
\] (2.23)

We now argue that since the measurable properties (such as resistance) of a metal are controlled by the density of states at the Fermi surface, changing the magnetic field will produce oscillations in those measurable properties. For instance, let the \(n^{th}\) orbit be near
the Fermi surface, if we shift the magnetic field such that the \((n + 1)\)th orbit now has the same \(\vec{k}\)-space orbit size, the orbits, and hence the density of states, around the Fermi surface should appear unchanged. Therefore, in magnetic fields that are strong enough to quantize orbits, we expect that the conductivity to oscillate as the density of states near the Fermi surface. This oscillation is known as the Shubnikov-de Haas effect. By requiring the same \(\vec{k}\)-space area for the \(n\)th and \((n + 1)\)th orbits, Eq. 2.23 tells us that the oscillations exhibit a period of \(1/B\). We will use the oscillations of the conductance in Chapter 4 to study the quantization transition induced by a magnetic field.
Chapter 3

Zener-tunneling and magnetoresistance in p-n junctions

We begin our discussion of relativistic dynamics in graphene with the simplest gated geometry, a single p-n junction. Graphene p-n junctions have been fabricated recently in locally gated samples [49, 50, 51] and provide a tool to study electron transport. As we mentioned before, charge carriers in graphene mimic relativistic Dirac particles with zero mass and linear dispersion relation $\varepsilon = \pm v_F|\vec{p}|$ with $v_F \approx 10^8$ cm/s. Graphene p-n junctions are predicted to exhibit signatures of chiral dynamics of massless Dirac particles: perfect transmission normal to the junction [11, 12] and collimation of the transmitted particles [13]. Ballistic transport in p-n junctions was proposed as a means to realize an electron lens [52].

The properties of the p-n-p system studied in Ref. [49] could be mainly explained by conduction in the disordered p and n regions, rather than in the p-n junctions. Likewise, the effects in quantizing magnetic fields [50, 51] were understood from edge state transport in the p and n regions, with the p-n interface merely providing mode mixing [53]. In neither of the experiments [49, 50, 51] the effects of ballistic transmission [11, 13, 52] seemed to stand out.

This is not too surprising, given that direct detection of the effects [11, 12, 13, 52] would require an angle-resolved measurement and/or very clean samples. Alternatively, one can ask if the behavior [11, 12, 13, 52] can be inferred from the dependence of transport properties on the magnetic field that often provides valuable insights into electron dynamics. It is
interesting therefore to better understand the signatures of ballistic transmission in external magnetic field, which is the main purpose of this chapter.

We start by noting that the coupling of an electron to external fields reflects relativistic character of charge carriers in graphene with the speed of light $c$ replaced by $v_F$. In relativistic electro-magnetic theory the fields $\vec{E}$ and $\vec{B}$ are treated on equal footing, playing the role of each other in a moving reference frame. The dynamics of a relativistic particle in uniform fields depends only on the Lorentz invariants $E^2 - B^2$, $\vec{E} \cdot \vec{B}$ [19]. In particular, the dynamics in crossed fields, $\vec{E} \cdot \vec{B} = 0$, can be of two main types, magnetic and electric, depending on the sign of $E^2 - B^2$. In the first case, $B > E$, the particle trajectories are described by cyclotron motion superimposed with a drift perpendicular to $\vec{L}$. In the second case, $E > B$, the trajectories are similar to those in the absence of $B$ field, moving asymptotically parallel to $\vec{E}$ and exhibiting no cyclotron motion.

Quantum transport in these two regimes, magnetic and electric, was discussed a while ago [54, 55] in the context of interband tunneling in two-band semiconductor systems modeled by the Dirac equation. Naturally, both of these regimes can be realized in graphene p-n junctions. In the magnetic case, realized for $B > (c/v_F)E$ [20], electron motion is described by quantized Landau levels with a linear dispersion in the momentum perpendicular to $\vec{E}$, i.e. parallel to the junction. This defines relativistic Quantum Hall edge states [56] transporting charge along the p-n interface. The cyclotron frequency in this regime as a function of $E$ vanishes at $E = (v_F/c)B$, signaling collapse of the Landau levels and Quantum Hall effect [20].

In the electric regime $B < (c/v_F)E$, which will be of main interest for us here, electrons can move freely along $\vec{E}$, transporting electric current through the junction. The transmission coefficient, found below as a function of $B$, is shown to vanish at the critical field

$$B = B_* \equiv (c/v_F)E.$$  \hspace{1cm} (3.1)

The effect of increasing magnetic field is therefore to pinch off transport through the junction, and transform it into the edge state transport along the junction in the Quantum Hall state at $B > B_*$. Similar conclusions for tunneling suppression by transverse mag-
Figure 3-1: Schematic of a p-n junction in a locally gated sample. For the geometry shown (wide and short sample) the conductance is dominated by the junction. Magnetic field suppresses conductance as $G(B) \propto (1 - (B/B_*)^2)^{3/4}$, Eq.(3.2).

In our approach, we solve the Dirac equation in crossed $E$ and $B$ fields exactly with the help of a Lorentz boost. This allows us to treat the monolayer and bilayer cases on equal footing. We find collimated transmission, as in the absence of magnetic field, but peaked at an angle $\sin \theta_B = B/B_*$, with unit transmission at the peak, $\theta = \theta_B$. The net conductance, found by integrating transmission over angles $\theta$, for a wide junction is given by

$$G(B \leq B_*) = \frac{e^2 w}{2\pi \hbar d} \left(1 - (B/B_*)^2\right)^{3/4}, \quad (3.2)$$

where $d = (\hbar v_F/|eE|)^{1/2}$ and $w$ is the p-n interface length (see Fig.3-1). The suppression of tunneling (3.2) precedes formation of edge states at the p-n interface at $B > B_*$.

To estimate the critical field $B_*$ for the parameter values of Refs.[49, 50, 51] one would have to account for screening of the in-plane field created by gates[57]. To bypass these complications, we assume that a density variation of order $n_0 \sim 10^{12}$ cm$^{-2}$ is created in a p-n junction across a distance $\ell \approx 50$ nm. Then the field felt by the electrons is $eE \sim \hbar v_F \sqrt{\pi n_0}/\ell$, giving

$$B_* = (c/v_F)E \sim (\hbar c/e) \sqrt{\pi n_0}/\ell. \quad (3.3)$$
In terms of the magnetic length $\ell_B = \sqrt{hc/eB}$, this translates into $\ell_B^2 = \ell / \sqrt{\pi n_0} \approx 260 \text{ nm}^2$, yielding an experimentally convenient value of $B \sim 2.5 \text{ T}$.

For the p-n junction contribution to dominate over the conduction in the p and n regions, it is beneficial to be in the ballistic regime, similar to Refs.[11, 13, 52], and to use wide and short samples (see Fig.3-1). These requirements are more relaxed for p-n junctions in epitaxial and bilayer systems, where tunneling is exponentially suppressed owing to the presence of a spectral gap (see below).

We first consider transport in the p-n junction in the absence of magnetic field. Massless Dirac particles in graphene moving near the p-n interface in a uniform in-plane electric field are described by the Hamiltonian

$$H = e\phi(\vec{x}) + v_F \begin{pmatrix} 0 & p_+ \\ p_- & 0 \end{pmatrix}, \quad p_{\pm} = p_1 \pm ip_2,$$

where $\phi$ is the electrostatic potential used to create the junction. Here, we adopt a relativistic notation where $x_1 = x$, $x_2 = y$, and eventually $v_F t = x_0$. We consider a p-n interface parallel to the x axis (Fig.3-1), with the external field $\vec{E} \parallel \hat{y}$ described by $\phi(\vec{x}) = -E x_2$.

The eigenstates of (3.4) are characterized by the momentum component parallel to the junction, $\psi(t, \vec{x}) = e^{-ipt}p_1 \psi(x_2)$, giving a 1D problem for $\psi(x_2)$. Following Ref.[66], we choose to write this problem in momentum representation

$$-ieE \frac{d\psi}{dp_2} = \tilde{H}\psi, \quad \tilde{H} = v_F(p_1\sigma_1 - p_2\sigma_2) - \epsilon.$$  \hspace{1cm} (3.5)

As noted in Ref.[66], momentum representation provides direct access to the asymptotic scattering states, and is thus more beneficial than the position representation.

Indeed, Eq.(3.5), interpreted as a time-dependent evolution with the Hamiltonian $\tilde{H}$, "time" $p_2$, and "Planck’s constant" $eE$, can be identified with the Landau-Zener problem for a two-level system evolving through an avoided crossing. Hence the probability to be transmitted (reflected) in the Dirac problem translates into the probability of a diabatic (adiabatic) Landau-Zener transition. The transmission coefficient can thus be found using
the answer for the latter [68], giving

$$T(p_1) = \exp(-\pi \hbar v_F p_1^2 / |E|),$$

(3.6)

which agrees with the results of [66, 13] (see also [67]).

Alternatively, the result (3.6) can be put in the context of Klein tunneling that links transmission of a Dirac particle through a steep barrier with electron/hole pair creation. The pair creation rate can be found as the probability of an interband transition occurring when the particle momentum evolves as $p_2 = eEt$. Because each created pair transfers one electron charge across the p-n interface, the pair creation rate is equal to the tunneling current.

To analyze transport in the p-n junction in the presence of a magnetic field, it will be convenient to rewrite the Dirac equation (3.4) in a Lorentz-invariant form

$$\gamma^\mu \left(p_\mu - a_\mu\right)\psi = 0, \quad \{\gamma_\mu, \gamma_\nu\}_+ = 2g_{\mu\nu},$$

(3.7)

where $\gamma^\mu$ are Dirac gamma-matrices, $\gamma^0 = \sigma_3$, $\gamma^1 = -i\sigma_2$, $\gamma^2 = -i\sigma_1$, and $\psi$ is a two-component wave function. Here we use the space-time notation for coordinates $x_\mu = (v_F t, x_1, x_2)$, momenta $p_\mu = h(i\gamma^{-1}_\mu \partial_{x_\mu} - i\partial_{x_1} - i\partial_{x_2})$, and external field $a_\mu = (a_0, a_1, a_2)$. The fields $\vec{E}$ $\parallel \vec{y}$ and $\vec{B}$ $\parallel \vec{z}$ are described by

$$a_0 = -\frac{e}{v_F} E_y, \quad a_1 = -\frac{e}{c} B_y, \quad a_2 = 0.$$

(3.8)

The Dirac equation (3.7) is invariant under the Lorentz group $(d = 2 + 1)$:

$$x'^\nu = \Lambda'^\nu_\mu x^\mu, \quad p'^\mu = \Lambda'^\mu_\nu p_\nu, \quad a'^\mu = \Lambda'^\mu_\nu a_\nu,$$

$$\psi' = S(\Lambda)\psi,$$

(3.9)

(3.10)

where $S(\Lambda) = \exp\left(\frac{i}{\hbar} \omega_{\mu\nu} [\gamma^\mu, \gamma^\nu]\right)$ for $\Lambda = \exp(\omega)$.

Before appealing to Lorentz invariance, we first find transmission quasiclassically, using the same factorization as above, $\psi(t, \vec{x}) = e^{-ict+i\mu p_1 x_1} \psi(x_2)$, which gives a 1D problem for
\[ \psi(x_2): \]
\[ (\gamma^0(\epsilon + ax) + \gamma^1(p_1 + bx) - i\gamma^2 \partial_x)\psi(x) = 0 \]  
\[ (3.11) \]

where \( a = \frac{\xi}{\hbar} E, \ b = \frac{\xi}{\hbar} B, \ x \equiv x_2 \). Eq.(3.11) can be cast in the form of evolution with a non-hermitian Hamiltonian:

\[ i\partial_x \psi(x) = ((\epsilon + ax)\sigma_2 + i(p_1 + bx)\sigma_3)\psi(x). \]  
\[ (3.12) \]

Now, we apply the adiabatic approximation, constructed in terms of \( x \)-dependent eigenstates and eigenvalues of the non-hermitian Hamiltonian. The eigenvalues are \( \pm \kappa(x) \), where \( \kappa(x) = \sqrt{(\epsilon + ax)^2 - (p_1 + bx)^2} \). This quantity is imaginary in the classically forbidden region \( x_1 < x < x_2 \), where \( x_{1,2} = (\epsilon \pm p_1)/(a \pm b) \). The WKB transmission coefficient then equals \( e^{-S} \), where

\[ S = 2 \int_{x_1}^{x_2} \text{Im} \kappa(x) dx = \pi \frac{(p_1 a - b \epsilon)^2}{(a^2 - b^2)^{3/2}}. \]  
\[ (3.13) \]

For \( B = 0 \) our WKB result (3.13) agrees with Eq.(3.6).

The problem (3.7), (3.8) can also be solved exactly with the help of a Lorentz transformation chosen so as to eliminate the field \( B \). (This is possible because the Lorentz-invariant combination \( \vec{B}\cdot\vec{E} \) equals zero.) For a not too large magnetic field, \( B < B_s = \frac{\xi}{\hbar} E \), we can eliminate \( B \) by a Lorentz boost with velocity parallel to the junction:

\[ \Lambda = \begin{pmatrix} \gamma & \gamma \beta & 0 \\ \gamma \beta & \gamma & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \gamma = \frac{1}{\sqrt{1 - \beta^2}} \]  
\[ (3.14) \]

Choosing the boost parameter as \( \beta = -\nu_{TF} B/cE = -B/B_s \), in the new frame we have \( B' = 0 \), \( E' = E/\gamma \).

Because \( B' = 0 \), the transmission coefficient for an electron with momentum \( p'_1 \) parallel to the p-n junction is given by \( T = e^{-\pi \nu_{TF} \nu' \kappa^2 \lvert \epsilon E \rvert} \) in the new frame (see Eq.(3.6) and [66, 13]). Expressing \( p'_1 \) and \( E' \) through the quantities in the lab frame, we obtain

\[ T(p_1) = e^{-\pi \gamma^2 d(p_1 + \beta \epsilon)^2}, \quad d = (\hbar \nu_{TF}/|\epsilon E|)^{1/2}, \]  
\[ (3.15) \]
\[ T(\theta) = e^{-\alpha \gamma^2 (\sin \theta - B/B_0)^2}, \text{Eq.}(3.15), \text{for } \alpha = \pi (d/\lambda_F)^2 = 20. \] Transmission reaches unity at a field-dependent angle \( \theta_B = \arcsin B/B_* \).

\( \epsilon = \epsilon/\nu_F \), which coincides with the WKB result (3.13).

In passing from the moving and lab frames we used the fact that the transmission coefficient \( T \), Eq.(3.15), is a scalar with respect to Lorentz transformations (3.14). This is true because transmission and reflection at the p-n interface is interpreted in the same way by all observers moving with the velocity parallel to the interface.

The dependence of the transparency (3.15) on the electric field \( E \) is such that \( T \) grows as \( E \) increases. This is a manifestation of the Klein tunneling phenomenon in which steeper barriers yield higher transmission.

The result (3.15) features exponential suppression of tunneling by \( B \) field for all momenta except \( p_1 = -\beta \epsilon \) that yields perfect transmission. This corresponds to the incidence angle \( \theta_B = \arcsin B/B_* \) (see Fig.3-2). At equal p and n densities, the velocities of transmitted particles are collimated at \( \theta \approx \theta_B \), with the collimation angle variance determined by \( \Delta p_1 \approx d^{-1} \gamma^{-3/2} \). This gives an estimate

\[
\Delta \theta \sim \left( \lambda/d \right) \left( 1 - (B/B_0)^2 \right)^{1/4}, \quad \lambda = v_F/\epsilon_F. \quad (3.16)
\]

We conclude that the nearly unit transmission, which occurs perpendicular to the p-n interface at \( B = 0 \) [11, 13], persists at finite magnetic fields, albeit for \( \theta_B \neq 0 \). This behavior of the collimation angle can be used to realize a switch (see Fig.3-3), in which current is
Figure 3-3: Field-controled switching of collimated current flow through a ballistic p-n junction between different contacts.

channeled between different pairs of contacts by varying the $B$ field.

The p-n junction net conductance can be found from the Landauer formula

$$G = \frac{e^2}{h} \sum_{-k_F < p_1 < k_F} T(p_1) = \frac{we^2}{2\pi h} \int_{-k_F}^{k_F} T(p_1) dp_1$$

(3.17)

where $w$ is the length of the junction interface (see Fig.3-1), and the states contributing to transport are those at the Fermi level, $\epsilon = \epsilon_f$. For a wide junction, $w \gg d \gg \lambda_F$, extending integration over $p_1$ to infinity we obtain the $(1 - (B/B_*)^2)^{3/4}$ dependence (3.2).

It is interesting to apply these results to epitaxial graphene, described by massive Dirac particles $\epsilon = \pm(v_F^2 p^2 + \Delta^2)^{1/2}$ with an energy gap $\Delta$ induced by the substrate [69, 70]. The generalization amounts to replacing $p_1^2$ by $p_1^2 + \Delta^2/v_F^2$ in (3.6). Performing Lorentz transformation, we find exponential suppression of conductance:

$$G(B) = \frac{e^2}{2\pi h} \frac{w}{d} (1 - \beta^2)^{3/4} \exp\left(-\frac{\pi d^2 \Delta^2}{\sqrt{2}\lambda_F (1-\beta^2)^{1/2}}\right)$$

(3.18)

(cf. Refs. [54, 55]). The angular dependence of transmission in this case is the same as in the massless case.

We note that $G(B \geq B_*) = 0$ does not necessarily mean that the system ceases to conduct. The behavior predicted by Eq.(3.2) at $B \geq B_*$ should be interpreted as 2D transport.
Figure 3-4: A comparison of the theoretical ballistic magnetoconductance (solid lines) (Eq. 3.2) with experimental data (dotted lines) from the supplemental material of Ref. [74] (sample C540). Parameters are taken from the same reference, with the junction length $\ell$ estimated to be 50 nm. As we can see, transport is not entirely ballistic and additional contributions exist in the data.

pinching off by the onset of the Quantum Hall effect. In that, just the part of the conductance proportional to the sample width $w$ vanishes, while the edge mode contribution remains nonzero. A comparison of our prediction for ballistic magnetoconductance with experimental data is provided in Figure 3-4. The sample in question contains non-ballistic contributions to conductance.

Our approach can be readily generalized to describe p-n junctions in graphene bilayers [39]. The bilayer Hamiltonian [2] includes the standard monolayer tight-binding part, as well as a direct coupling between the adjacent sites $B_2, A_1$ of different monolayers and a weaker coupling between non-adjacent sites $A_2, B_1$: $\gamma_{B_1A_2} < \gamma_{B_2A_1} \approx 0.4$ eV in notation of Ref.[2]. Here, for simplicity, we ignore $\gamma_{B_1A}$ and denote $\gamma_{B_1A}$ as $\Delta$.

It is convenient to write the bilayer Hamiltonian, linearized near the Dirac points, in pseudospin notation, using $\tau_3 = \pm 1$ to label the monolayers. The inter-layer coupling takes the form $H_A = \Delta (\tau_+ \sigma^- + \tau_- \sigma^+) = \Delta 4 (\tau_1 \sigma_1 + \tau_2 \sigma_2)$, where $\sigma_\pm = \frac{1}{2} (\sigma_1 \pm i \sigma_2)$, $\tau_\pm = \frac{1}{2} (\tau_1 \pm i \tau_2)$. This gives the Hamiltonian

$$H = v_F p_1 \sigma_1 - v_F p_2 \sigma_2 + \frac{1}{2} u \tau_3 + \frac{\Delta}{2} (\tau_1 \sigma_1 + \tau_2 \sigma_2),$$

(3.19)
where \( u \) is the vertical field that opens a gap of size \( |u| \) in the bilayer spectrum. Multiplying the time-dependent Schrödinger equation by \( \sigma_3 \), we rewrite it as a Dirac equation (3.7) with a fictitious \( \tau \)-dependent gauge field:

\[
\gamma^\mu(p_\mu - a_\mu - g_\mu)\psi = 0, \quad g_\mu = (\tilde{\mu}\tau_3, -\tilde{\Lambda}\tau_1, \tilde{\Lambda}\tau_2),
\]

(3.20)

where \( \tilde{u} = u/2v_F \), \( \tilde{\Lambda} = \Delta/2v_F \), and the external field \( a_\mu \) is defined in the same way as above.

Under Lorentz boost (3.14) the equation \( \gamma^\mu(p_\mu - a_\mu - g_\mu) = 0 \) changes covariantly with the momenta and fields transforming via \( p' = \Lambda p, \ a' = \Lambda a, \ g' = \Lambda g \), giving \( g_\mu = \frac{1}{2v_F} (\gamma(u\tau_3 - \beta\Delta\tau_1), \gamma(\beta\mu\tau_3 - \Delta\tau_1), \Delta\tau_2) \). Choosing \( \beta \) so as to eliminate the \( B \) field, we find the transformed Hamiltonian \( H' = -eE'x_2 + H_k(p'_1, p'_2) \), where

\[
H_k(p'_1, p'_2) = \frac{1}{2} \gamma(u\tau_3 - \beta\Delta\tau_1) + \\
\left( v_Fp'_1 - \frac{1}{2} \gamma(\beta\mu\tau_3 - \Delta\tau_1) \right) \sigma_1 - \left( v_Fp'_2 - \frac{1}{2} \Delta\tau_2 \right) \sigma_2.
\]

(3.21)

Working in the momentum representation, as above, we treat \( e'\psi' = H'\psi' \) as a first-order differential equation

\[
ieE'\frac{d\psi}{dp'_2} = (H_k(p'_1, p'_2) - e')\psi.
\]

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We evaluate the transfer matrix of this equation numerically, and find that in the physically interesting case $u \ll \Delta$, the lowest and the uppermost energy levels of $H_k$ are decoupled from the two middle levels. The $4 \times 4$ transfer matrix is thus reduced to a $2 \times 2$ matrix, yielding the transmission and reflection coefficients.

Transmission features an interesting behavior as a function of external fields and particle momentum (see Fig.3-5). It has a symmetric double hump profile as a function of $p_1$ and $u$ vanishing between the humps (unlike single gaussian peak in the monolayer case) and, somewhat unexpectedly, perfect transmission at the peak. At large $p_1$ and $u$, because of the energy gap opening, transmission is strongly suppressed. Conductance, found from the Landauer formula (3.17), also exhibits strong suppression at increasing $u$ and $B$, qualitatively similar to the gapped monolayer case, Eq.(3.18).

To summarize, we have seen Klein tunneling derived in a monolayer p-n junction with a few methods, including an appeal to Lorentz symmetry. We find that Klein tunneling is preserved in magnetic field, but the angle of transmission is deflected. The ballistic conductance pinches off at a critical magnetic field that corresponds to the transition between spacelike and timelike quality of the Lorentz scalar $\sqrt{\vec{E}^2 - \vec{B}^2}$. Physically, this boundary separated the continuous spectrum in low $B$ field from the quantized energy levels of the Quantum Hall effect in high $B$. We also use the same technique on bilayer graphene to derive a transmission profile that demonstrates anti-Klein tunneling.
Chapter 4

Landau level collapse in gated graphene

We describe a new regime of magnetotransport in two dimensional electron systems in the presence of a narrow potential barrier. In such systems, the Landau level states, which are confined to the barrier region in strong magnetic fields, undergo a deconfinement transition as the field is lowered. Transport measurements on a top-gated graphene device are presented. Shubnikov-de Haas (SdH) oscillations, observed in the unipolar regime, are found to abruptly disappear when the strength of the magnetic field is reduced below a certain critical value. This behavior is explained by a semiclassical analysis of the transformation of closed cyclotron orbits into open, deconfined trajectories. Comparison to SdH-type resonances in the local density of states is presented.

Electron cyclotron motion constrained by crystal boundaries displays interesting phenomena, such as skipping orbits and electron focusing, which yield a wealth of information on scattering mechanisms in solids [58, 59]. Since the 1980s, semiconducting two-dimensional electron systems (2DES) have become a vehicle for investigating the interplay between gate-induced potential and cyclotron motion. A variety of interesting phenomena were explored in these systems, including quenching of the quantum Hall effect [60, 61], Weiss oscillations due to commensurability between cyclotron orbits and a periodic grating [62], pinball-like dynamics in 2D arrays of scatterers [63], and coherent electron focusing [64].

The experimental realization of graphene [1], a new high-mobility electron system, affords new opportunities to explore effects that were previously inaccessible. Here we
focus on one such phenomenon, the transformation of the discrete Landau level spectrum to a continuum of extended states in the presence of a static electric field. Previous attempts to induce sharp potential barriers in III-V semiconductor structures have been limited by the depth at which the 2DES is buried—typically about 100 nm below the surface\cite{65}. In contrast, electronic states in graphene, a truly two-dimensional material, are fully exposed and thus allow for potential modulation on ~ 10 nm length scales using small local gates and thin dielectric layers\cite{49, 50, 51, 32}.

To probe the phenomena of interest, barrier widths must be comparable to the magnetic length $\ell_B = (\hbar c/eB)^{1/2}$ for the fields in which magnetic oscillations can be observed. This condition gives characteristic fields as low as 30 mT for systems such as GaAs. Magnetic oscillations are nearly washed out at such fields, making the effects described below hard to probe in GaAs structures. In contrast, the gate widths available in graphene translate to much higher fields of a few Tesla, making graphene the system of choice for this experiment.

The behavior which will be of interest for us is illustrated by a toy model involving the Landau levels of a massive charged particle in the presence of an inverted parabolic potential $U(x) = -ax^2$. Competition between the repulsive potential and magnetic confinement gives rise to a modified harmonic oscillator spectrum

$$
\varepsilon_n(p_y) = \frac{\hbar e}{m} \sqrt{B^2 - B_c^2} (n + 1/2) - \frac{2ap_y^2}{e^2(B^2 - B_c^2)}
$$

(4.1)

for $B > B_c$, where $m$ is the particle mass, $p_y$ is the $y$ component of momentum, and $B_c = \sqrt{2ma/e}$ is the critical magnetic field strength. For strong magnetic field, $B > B_c$, the spectrum consists of discrete (but dispersive) energy bands indexed by an integer $n$, whereas for $B \leq B_c$ the spectrum is continuous even for fixed $p_y$. This behavior can be understood quasiclassically in terms of transformation of closed cyclotron orbits into open orbits, which occurs when the Lorentz force is overwhelmed by the repulsive barrier potential.

Landau levels of massless Dirac charge carriers in single-layer graphene, subject to a
linear potential $U(x) = -eEx$, exhibit an analogous collapse of the discrete spectrum [20]:

$$\epsilon_n(p_y) = \pm v_F \sqrt{2n\hbar eB} \left(1 - \beta^2\right)^{3/4} - \beta v_F p_y,$$

(4.2)

where $n = 0, 1, 2...$ and $\beta = E/v_FB$. The transition at $B_c = E/v_F$ can be linked to the classical dynamics of a massless particle, characterized by closed orbits at $B > B_c$ and open trajectories at $B < B_c$ [21].

A simple picture of the spectrum (4.2) can be obtained from the Bohr-Sommerfeld (BS) quantization condition

$$\int_{x_1}^{x_2} p_x(x)dx = n\hbar(n + \gamma),$$

(4.3)

where $x_1$ and $x_2$ are the turning points, $\gamma = 0$ due to the Berry phase contribution for Dirac fermions, and

$$p_x(x) = \sqrt{\left(\epsilon - U(x)\right)^2/v_F^2 - (p_y - eBx)^2}.$$

(4.4)

For linear $U(x)$, this gives the Landau level spectrum (4.2) for $B > B_c$. As $B$ approaches $B_c$, one of the turning points moves to infinity, indicating a transformation of closed orbits into open trajectories.

To realize the collapse of Landau levels in an electron system, several conditions must be met. First, it must be possible to create a potential barrier that is steep on the scale of the cyclotron orbit radius. Second, the system must be ballistic on this length scale, in order to suppress the broadening of Landau levels due to disorder. Graphene, which is a truly two-dimensional material with high electron mobility, fulfills both conditions. Crucially, as demonstrated by the recent observation of Fabry-Perot (FP) oscillations in gated graphene structures [32], transport can remain ballistic even in the presence of a gate-induced barrier. Thus graphene is an ideal system for studying the Landau level collapse.

Transport data taken from a locally gated device similar to that described in Ref.[32] are shown in Fig.4-1. Graphene was prepared via mechanical exfoliation and contacted using electron beam lithography before being coated with a 7/10 nm thick hydrogen silsesquioxane/HfO₂ dielectric layer. Narrow (~16 nm) palladium top gates were then deposited, and the electri-
Figure 4-1: (a) Differentiated conductance, $dG/dV_{tg}$, of a narrow top gate graphene device, pictured in (c). Fabry-Perot (FP) oscillations appear in the presence of confining pn junctions. (b) $dG/dV_{tg}$ as a function of $B$ and $V_{tg}$. Shubnikov-de Haas (SdH) oscillations are observed at high $B$. The fan-like SdH pattern is altered by the barrier: in the pp’p region it curves, weakens, and is washed out at fields $|B| \lesssim B_c$, Eq.(4.7), while in the pnp region a crossover to FP oscillations occurs. Data shown correspond to $V_{bg} = -70$V [dashed line in (a)]. (c) Top gated graphene device micrograph and schematic; top gate width is $\sim 16$nm. (d) Local density of states (DOS) in the middle of parabolic barrier. The energy derivative $dN/d\epsilon$ [see Eq.(4.10)], which corresponds to the measured quantity $dG/dV_{tg}$, is shown. Dashed parabola marks the critical field, Eq.(4.8). Oscillations in the DOS modulate the rate of scattering by disorder, resulting in the SdH effect [72].
Figure 4-2: (a) Traces of the conductance data from Fig.4-1b for several magnetic field values. Landau level numbers are shown next to the corresponding peaks. The SdH oscillations abruptly disappear in the unipolar (pp'p) region as the magnetic field is lowered to \( B \approx 3 \) T, and yet persist to much lower fields in the pnp region. (b) Traces of the calculated local DOS (see Fig.4-1d) showing similar behavior. The traces are artificially offset from each other for visual clarity. In both plots, as the magnetic field is lowered, higher number Landau Levels collapse first, indicating a dependence of the critical field \( B_c \) on energy/gate voltage.

The resistance measured at 1.6 Kelvin. Finite element modeling[32] yields density profile

\[ e \rho(x) \approx \frac{C_{tg} V_{tg}}{1 + x^2/w^2} + C_{bg} V_{bg}, \]  

(4.5)

with \( w \approx 45 \) nm, where \( C_{tg(bg)} \) and \( V_{tg(bg)} \) are the top (bottom) gate capacitance and applied voltage. To subtract the series resistances of the graphene leads, the numerical derivative of the conductance with respect to the top gate voltage, \( dG/dV_{tg} \), was analyzed.

At zero magnetic field (Fig.4-1a), \( dG/dV_{tg} \) shows distinct behavior in four regions in the \((V_{bg}, V_{tg})\) plane, corresponding to pp'p, pnp, npn, and nn'n doping, where n (p) refers to negative (positive) charge density and prime indicates different density. The appearance of FP interference fringes when the polarity of charge carriers in the locally gated region and graphene leads have opposite signs indicates that the mean free path is comparable to the barrier width, \( l_{mf} \sim w \).

In high magnetic field, a fan of SdH resonances corresponding to Landau levels is seen in both the bipolar and unipolar regimes (see Fig.4-1b). At lower fields, the observed behavior depends on the polarity under the gate. In the bipolar regime, as \( B \) is lowered, the
SdH resonances smoothly evolve into FP resonances. The half-period shift, clearly visible in the data at $B \approx 1$ T, is a hallmark of Klein scattering [25]. In the unipolar regime, the SdH resonances bend, becoming more horizontal at lower field. The oscillations first begin to lose contrast, and then completely disappear below $B_c \approx 4$ T (Fig. 4-2).

The connection between this behavior and Landau level collapse is exhibited most clearly by a semiclassical analysis. The SdH resonances arise from an oscillatory contribution to the density of states at the Fermi level due to closed trajectories; the BS condition (4.3) with $\epsilon = \epsilon_F$ and $p_y = 0$ gives a good estimate for the positions of those resonances. For a generic barrier potential, Eq. (4.3) can be written directly in terms of experimental control parameters. Using the Thomas-Fermi approximation, and ignoring the effects of ‘quantum capacitance’ and nonlinear screening [71], we define the position-dependent Fermi momentum $k_F(x) = \sqrt{4\pi \rho(x)/g}$, where $g = 4$ is the spin/valley degeneracy. Substituting the relation $\epsilon - U(x) = \hbar \nu F k_F(x)$ into Eq. (4.4), we obtain

$$\int_{x_1}^{x_2} \frac{4\pi}{g} \frac{\hbar^2 \rho(x) - (p_y - eBx)^2}{dx} = \pi \hbar(n + \gamma). \tag{4.6}$$

Interestingly, and somewhat unexpectedly, the quantization condition assumes the same form for massless and massive carriers with $g = 4$ (monolayer and bilayer graphene); it would thus be trivially modified for GaAs quantum wells ($g = 2$ and $\gamma = 1/2$).

A rough estimate for the critical field can be obtained by comparing the curvature of $\rho(x)$ at $x = 0$ with the $B^2 x^2$ term in Eq. (4.6). Near the polarity reversal boundary $C_{bg} V_{bg} + C_{tg} V_{tg} = 0$ (white dashed line in Fig. 4-1a), using the device parameters $C_{bg} = 115 \text{ aF/}\mu\text{m}^2$, $V_{bg} = -70$ V, $w = 50$ nm, we find $B_c = (\hbar/e w) (\pi C_{bg} V_{bg}/e)^{1/2} \approx 5.2$ T.

The dependence of $B_c$ on experimental control parameters $V_{tg}$ and $V_{bg}$ can be obtained by analyzing the turning points for the density profile (4.5). Setting $p_y = 0$ gives $\hbar k_F(x) = \pm eBx$. Solving this equation and equating the result to barrier half-width, $x_{1(2)} = \pm w$, we obtain

$$B_c = (\hbar/e w) \sqrt{(2\pi/eg)(2C_{bg} V_{bg} + C_{tg} V_{tg})}. \tag{4.7}$$

Both the value of $B_c$ and its dependence on gate voltages matches the data quite well (red
The actual density profile is nonparabolic, flattening outside the top gate region (TGR) on a length scale $2w \approx 100\text{ nm}$. Yet, since the magnetic length $\ell_B$ is much shorter than $2w$ for the fields of interest ($B \gtrsim 1\text{ T}$), this flattening does not significantly impact our discussion of the collapse phenomenon. While the states realized at subcritical magnetic fields are not truly deconfined due to cyclotron motion in the region outside the TGR, the corresponding orbits are very long. For such states, the particle traverses the TGR, makes a partial cyclotron orbit outside of the TGR, and finally crosses the TGR again to close the orbit (Fig.3a). The net orbit length is a few $w$, which is much greater than the orbit size at strong fields (a few $\ell_B$). The contribution of long orbits to SdH oscillations will be suppressed due to spatial inhomogeneity and disorder scattering; hence the distinction between confined and deconfined orbits remains sharp despite the flattening of the potential (also, see a more detailed discussion in Appendix A).

With that in mind, below we analyze a simple model, $U(x) = -ax^2$. A simple estimate of the collapse threshold can be obtained by considering balance between the Lorentz force and the force due to the electric field, $v_FB = -dU/dx$. This condition is satisfied for a particle moving parallel to the barrier with $x = \pm \ell$, $\ell = e v_FB/(2a)$. This gives an energy-dependent critical field,

$$B_\epsilon(\epsilon) = (2/ev_F) \sqrt{-ae},$$

which increases with detuning from neutrality, as in experiment.

We treat the problem using microscopic Hamiltonian

$$H = \begin{pmatrix} U(x) & v_F p_- \\ v_F p_+ & U(x) \end{pmatrix}, \quad p_\pm = -i\hbar \frac{d}{dx} \pm i(p_y - eBx),$$

where $p_y$ is the conserved canonical momentum component parallel to the barrier. We nondimensionalize the problem using “natural units”

$$\epsilon_* = (\hbar^2 v_F^2 a)^{1/3}, \quad x_* = \left(\frac{v_F \hbar}{a}\right)^{1/3}, \quad B_* = \frac{\hbar}{e} \left(\frac{a}{v_F \hbar}\right)^{2/3}. \quad \text{51}$$
For each value of $p_y$ and magnetic field $B$, we represent the Hamiltonian as an $M \times M$ matrix defined on a grid in position space, with periodic boundary conditions. We use the eigenvalues and eigenstates obtained from diagonalization to evaluate the local density of states (DOS) in the middle of the barrier,

$$N(\epsilon) = \int \frac{dp_y}{2\pi} \sum_{n=1}^{M} \frac{\Gamma}{\pi} \frac{\langle |\psi_{n,p_y}(x=0)|^2 \rangle}{(\epsilon - \epsilon_n)^2 + \Gamma^2},$$

(4.10)

with Landau level broadening incorporated through the Lorentzian width $\Gamma = 0.2\epsilon_*$. In our simulation, a system of size $L = 15x_*$ discretized with $M = 1500$ points was used. Averaging with a gaussian weight was used to suppress the effect of spurious states arising due to a vector potential jump at the boundary,

$$\langle |\psi_{n,p_y}(x=0)|^2 \rangle = \int dx' e^{-x'^2/2\sigma^2} |\psi_{n,p_y}(x')|^2,$$

(4.11)

with $\sigma \approx x_*$. Oscillations in the density of states (4.10) modulate the rate of electron scattering by disorder, and thus show up in transport quantities measured as a function of experimental control parameters, as in the canonical SdH effect [72].

The resulting local DOS exhibits oscillations which track Landau levels at high $B$ (Fig.4-1d). In the pp'p case, at lower $B$, discrete Landau levels give way to a continuous spectrum in the region inside a parabola (dashed line) which marks the collapse threshold, Eq.(4.8).

The DOS exhibits FP fringes in the pnp region at low $B$, however without the the half-period shift seen in $dG/dV_{tg}$ at $B \leq 1T$ (Fig.4-1). As discussed in Ref.[25], this half-period shift results from FP interference due to Klein scattering at pn interfaces. A proper model of this effect must account for ballistic transport in the system.

The collapse observed in the density of states is related to deconfinement of classical orbits. The orbits can be analyzed as constant energy trajectories of the problem

$$\epsilon = v_F \sqrt{p_x^2 + \tilde{p}_y^2} + U(x), \quad \tilde{p}_y = p_y - eBx.$$

(4.12)

For parabolic $U(x) = -ax^2$ the orbits with $p_y = 0$ can be easily found in polar coordinates.
Figure 4-3: (a) Closed orbits for the Thomas-Fermi potential obtained from the density profile, Eq.(4.5), with $B = 9, 7, 5, 3, 1$ T and $p_y = 0$. Long trajectories, extending far outside the gated region, do not contribute to SdH oscillations (see text). (b,c) Trajectories for the potential $U(x) = -ax^2$ and $p_y = 0$. Three types of trajectories are shown in momentum space (b) and position space (c): subcritical (red), critical (black), and supercritical (blue). The saddle points in momentum space correspond to motion along straight lines $x = \pm \ell$, where the Lorentz force is balanced by the electric field.

\[ p_x + ip_y = |p|e^{i\theta}: \]

\[
\frac{|p|}{p_0} = \frac{1}{\sin^2 \theta} \left( 1 \pm \sqrt{1 - \frac{\epsilon}{\epsilon_c} \sin^2 \theta} \right), \quad \epsilon_c = \frac{(v_F e B)^2}{4a} \tag{4.13}
\]

with $p_0 = v_F e^2 B^2 / 2a$ (see Fig.4-3b). Only real, positive solutions should be retained; when $\epsilon / \epsilon_c > 1$, the discriminant in Eq.(4.13) is negative near $\theta \approx \pi/2$ and trajectories cannot close (blue curves in Fig.4-3b).

The related orbits in position space can be found from the relation $dy/dx = \dot{y}/\dot{x} = \bar{p}_y/p_x$, giving

\[
\frac{dy}{dx} = \frac{\pm v_F (p_y - eBx)}{\sqrt{(\epsilon - U(x))^2 - v_F^2 (p_y - eBx)^2}}. \tag{4.14}
\]

For $p_y = 0$, integration is performed using the variable $u = x^2 / \ell^2$,

\[
\frac{y}{\ell} = \pm \int \frac{du}{\sqrt{(u + \epsilon / \epsilon_c - 2)^2 + 4(\epsilon / \epsilon_c - 1)}}, \tag{4.15}
\]

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where $\ell = v_F e B / 2a$ such that $\epsilon_c = a \ell^2$. The integrand changes its behavior at the critical energy $\epsilon_c$. For $\epsilon > \epsilon_c$, the integrand is real valued for all $u$ and

$$\sinh \left( \frac{y(x) - y_0}{\ell} \right) = \frac{x^2 / \ell^2 + \epsilon / \epsilon_c - 2}{2 \sqrt{\epsilon / \epsilon_c - 1}}. \quad (4.16)$$

For $\epsilon < \epsilon_c$, real solutions are divided into two domains $0 \leq u \leq 2 - \epsilon / \epsilon_c - 2 \sqrt{1 - \epsilon / \epsilon_c}$ (closed orbits) and $u > 2 - \epsilon / \epsilon_c + 2 \sqrt{1 - \epsilon / \epsilon_c}$ (open orbits):

$$\cosh \left( \frac{y(x) - y_0}{\ell} \right) = \pm \frac{2 - \epsilon / \epsilon_c - x^2 / \ell^2}{2 \sqrt{1 - \epsilon / \epsilon_c}}. \quad (4.17)$$

The red curves in Fig.4-3c correspond to the low energy regime, $\epsilon < \epsilon_c$, where orbits can either be closed (Landau levels) or open (trajectories for particle moving far from the barrier). At higher energies, $\epsilon > \epsilon_c$, all trajectories are open. The straight black lines correspond to the critical orbits of Eq.(4.8), where the Lorentz force and electric field are balanced. In addition to the two particular critical trajectories shown, in the limit $\epsilon / \epsilon_c \to 1$ there is an entire family of critical trajectories which asymptotically approach these lines.

Interestingly, unlike in the case of the potential obtained from the Thomas-Fermi model, where the classical turning points move continuously to infinity as the transition is approached, trajectories in the parabolic potential are trapped between the critical separatrix lines. At very low energies, closed orbits are approximately circular; as the energy increases towards $\epsilon_c$, orbits become more and more elongated, until finally merging with the separatrix at $\epsilon = \epsilon_c$ (see Fig.4-3).

In summary, graphene devices with a barrier induced by a narrow top gate can be used to probe electronic states on the spatial scale of a few tens of nanometers. In our transport measurements, the SdH-type resonances arising from quantized states associated with closed orbits are used to directly observe the competition between magnetic confinement and deconfinement due to electric field. As a result of this competition, the discrete spectrum of Landau levels collapses when subjected to a strong external potential. Experimental observations are found to be in good agreement with theory.
Chapter 5

Chirality-assisted confinement in bilayer p-n-p junctions

We demonstrate that a set of confined states exist in bilayer graphene with a p-n-p junction. These states are completely decoupled from the extended states outside of the junction due to chirality mismatch at the boundary. These states affect transport measurements directly, since normally incident electrons are reflected. In particular, the ballistic conductance shows a distinct non-Lorentzian line shape with a square root dependence on the gate voltage near resonance, with, in general, asymmetric coefficients on each side of the resonance. We also discuss the effects of an interlayer gap, which serves to round out the square root cusp.

Charge carriers in graphene have a number of interesting properties originating from their relativistic-like character [73]. Some of the most peculiar features are due to the chiral nature of electronic states, described by a $2 \times 2$ massless Dirac Hamiltonian with the two-component spinor wavefunction describing amplitudes on sublattices A and B. Eigenstates of such a Hamiltonian have their pseudospin locked by an effective momentum-dependent ‘magnetic field’, which makes particle velocity and pseudospin correlated in a specific way.

The chirality of electronic states manifests itself in some of the basic transport properties. In particular, chirality results in a Berry phase, given by $\pi$ in single-layer graphene (SLG) and $2\pi$ in bilayer graphene (BLG), that changes the character of cyclotron motion and gives rise to unconventional quantum Hall effects [7, 23, 26]. Another striking con-
sequence of chirality is ‘Klein tunneling’ featured by charge carriers transmission through potential barriers. Conservation of chirality requires that particles normally incident on a barrier in SLG cannot backscatter. As a result, the transmission at normal incidence equals unity independent of the barrier width, height or shape [76, 13, 74, 75]. Interesting manifestations of Klein tunneling in SLG can be seen in Fabry-Pérot (FP) resonances observed in transport measurements on gate-defined p-n-p heterojunctions. In particular, the conductance shows a periodic fringe pattern that undergoes a distinct half-period shift when a low magnetic field is imposed [77, 32].

Here we consider manifestations of chirality in transport through potential barriers in BLG. As we will see, while these manifestations are as dramatic as in SLG, they are of a totally different character, and under certain conditions lead to total backreflection of normally incident waves and spatial confinement. Because such behavior is in a certain sense opposite to that studied in SLG, it warrants a name ‘anti-Klein tunneling’. The Hamiltonian that governs transport through a barrier described by potential \( U(x) \), which is spatially uniform in the \( y \)-direction, is of the form [26]

\[
H = \begin{pmatrix}
U(x) & -\frac{\hbar^2}{2m} \left( \frac{d}{dx} + q \right)^2 \\
-\frac{\hbar^2}{2m} \left( \frac{d}{dx} - q \right)^2 & U(x)
\end{pmatrix},
\]

(5.1)

where \( m \approx 0.04 m_e \) is the BLG band mass and \( q \) is the wavevector \( y \) component. Normally incident electronic states which are described by \( q = 0 \), can be conveniently analyzed in the basis \( \frac{1}{\sqrt{2}} \left( \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right) \), \( \frac{1}{\sqrt{2}} \left( \begin{pmatrix} 1 \\ -1 \end{pmatrix} \right) \). In this basis the problem decouples into two Schrödinger equations of a canonical form:

\[
\left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \pm \left( U(x) - \epsilon \right) \right) \psi_{\pm}(x) = 0.
\]

(5.2)

For a special case of a potential step \( U(x \to -\infty) = U_1, U(x \to +\infty) = U_2 \), standard analysis shows that for particle energies in the interval \( U_1 < \epsilon < U_2 \) the left/right matching conditions couple propagating plane wave states on one side with evanescent states on the other side. Thus, the carriers normally incident on a potential step undergo total reflection, while the carriers incident at oblique angles have non-zero transmission probability.

Generalizing this analysis, below we show that potential barriers in BLG enable spatial
Figure 5-1: (top) The transmission probability and (bottom) the conductance numerically calculated using the gapless Hamiltonian, Eq.(5.1) with $U(x) = \frac{1}{2} m \omega^2 x^2$. The visible resonances in conductance correspond to the $\epsilon = \frac{1}{2} \hbar \omega$ and $\frac{3}{2} \hbar \omega$ harmonic oscillator bound states. Both resonances feature the characteristic square-root singularity $\delta G \propto -\sqrt{\phi \epsilon}$. Units are given in terms of $G_* = G_0 W/\ell$, where $W$ is the width of the sample. (Inset) A zoom in of the $\epsilon = \frac{1}{2} \hbar \omega$ resonance overlaid with 10 transmission profiles, with $q\ell$ changing between 0 and 0.18. Note that as $q$ increases, the resonance width increases. The almost horizontal (green) line is the background transmission, given for $q = 0$. The resonances display an asymmetric lineshape, described by a Fano model, with large $a$ [see Eq.(5.4)]. The transmission builds up on one side of this particular resonance, creating the inverted half-cusp [see Fig. 5-2] for $\epsilon < \frac{1}{2} \hbar \omega$. 
confinement of electronic states. We will construct states which are confined under barrier and have zero coupling to the continuum of states outside the barrier. The presence of such chirality-induced confined states manifests itself through FP-type resonances in transmission with the width of the resonances vanishing at normal incidence, \( q = 0 \). The infinite sharpness of these resonances at \( q = 0 \) results in singular peaks in conductance with unusual lineshapes, \( \delta G(\epsilon) \propto -\sqrt{|\epsilon - \epsilon_c|} \), where \( \epsilon_c \) is the position of the FP resonance. This behavior is clearly seen in the conductance in Fig. 5.1.

We will begin by identifying the confined states at normal incidence. Without loss of generality, we will work with parabolic potential \( U(x) = \frac{1}{2} m \omega^2 x^2 \). Setting \( q = 0 \) and separating the problem as in Eq.(5.2), we see that the equation with a plus sign describes Schrödinger particle in the presence of a binding parabolic potential. In this case, \( \psi_+(x) \) describes bound states confined inside a parabola. For a parabolic potential the energies of these confined states are

\[
\epsilon_n = h\omega(n + 1/2), \quad (n = 0, 1, 2...).
\]  

(5.3)

In contrast, Eq.(5.2) with the negative sign describes a particle subject to a potential barrier. Hence, in this case, \( \psi_-(x) \) describes continuum states with energies \(-\infty < \epsilon < +\infty\) that exist outside the barrier.

In order to discuss transmission, it is instructive to make connection to the standard framework of resonant tunneling. Crucially, transmission through the barrier is controled by different effects at zero \( q \) and at nonzero \( q \). At zero \( q \), the confined states are completely decoupled from the states in continuum, and thus the only mode of transmission available at \( q = 0 \) is tunneling through the barrier, described by the Schrödinger equation for \( \psi_-(x) \) which takes the form of an evanescent wave under the barrier. In contrast, at nonzero \( q \) the confined states acquire finite lifetime due to coupling to the continuum. Thus, in this regime transport is described by a resonant tunneling model with the width of the resonances being a function of \( q \) that vanishes at \( q = 0 \).

Since both evanescent and resonant transmission pathways are available at nonzero \( q \), interference between the two in general is described by a Fano-type model, where the
The transmission probability is given by:

\[
T(\epsilon) = \frac{1}{1 + a^2} \frac{(\epsilon - \epsilon_s)^2 + a\gamma}{(\epsilon - \epsilon_s)^2 + \gamma^2},
\]

(5.4)

with energy width \(\gamma\) and ‘asymmetry parameter’ \(a\) [78]. However, as we will now show, the evanescent contribution (direct tunneling) is always small and \(a\) large. In this case, the transmission is well approximated by the Breit-Wigner Lorentzian profile, which accounts for resonant transmission mediated by the confined state.

The Fano asymmetry parameter can be calculated as follows. For a potential with inversion symmetry, \(U(x) = U(-x)\), we can use the general relation derived in Ref.[79], \(a = |r_{bg}/t_{bg}|\), where \(r_{bg}\) and \(t_{bg}\) are the background reflection and transmission amplitudes in the absence of the resonance. For a wide barrier, such that the barrier width is larger than the Fermi wavelength, the tunneling transmission is exponentially small, yielding a large value for the parameter \(a\). In particular, for a parabolic barrier the exact expressions for the transmission and reflection coefficient[80] give \(|r_{bg}/t_{bg}| = \exp (\pi \epsilon/\hbar \omega)\). Even for \(\epsilon = \frac{1}{2} \hbar \omega\), \(a\) is large enough to justify the Lorentzian approximation, as seen in Fig. 5-1 (inset). This conclusion is in agreement with numerics, where the \(|t_{bg}| = 0.2\) is fairly small.

Transmission for our problem can be found by solving numerically the equations obtained from the Hamiltonian Eq.(5.1). Using the same basis as in the above analysis, and generalizing Eq.(5.2) to nonzero \(q\), we obtain two coupled equations

\[
\left[ -\frac{d^2}{dx^2} - q^2 + \frac{U(x) - \epsilon}{\hbar^2/2m} \right] \psi_z = \left[ 2q \frac{d}{dx} \pm \frac{mE_g}{\hbar^2} \right] \psi_\pm,
\]

(5.5)

where we also added an interlayer gap parameter via \(H_{gap} = H + \frac{E_g}{2} \sigma_3\). By solving these equations, we can find transmission \(t(\epsilon, q)\) as a function of energy and parallel wavevector, and evaluate conductance

\[
G(\epsilon) = G_0 W \int dq |t(\epsilon, q)|^2, \quad G_0 = N \frac{e^2}{2\pi \hbar},
\]

(5.6)

where \(W\) is the width of the sample in the \(y\)-direction, and \(N = 4\) is the spin/valley degeneracy of BLG. The integral in the expression for conductance, Eq.(5.6), runs over the interval
\(-k_F < q < k_F\), where \(k_F\) is the Fermi wavevector in the leads.

We now return to the discussion of the resonant tunneling model, and will describe the results of numerical analysis later. We see immediately that for small values of \(q\) and \(E_g\), the coupling between the confined and extended states, described by \(\psi_+\) and \(\psi_-\), is linear in \(q\) and \(E_g\) for small \(q\) and \(E_g\). Thus, in this regime the width of the resonance associated with the confined state is of order \(q^2\) or \(E_g^2\). For now, we will specialize to the case of \(E_g = 0\) for simpler analysis and restore nonzero gap later in our numerical simulations.

Hence, the contribution of a single quasibound state to transmission can be written in the Breit-Wigner Lorentzian approximation as

\[
tt(\epsilon, q) = \frac{\gamma(q)}{\gamma(q) + i(\epsilon - \epsilon_0(q))},
\]

where the parameters \(\epsilon_0(q)\) and \(\gamma(q)\) describe the resonance center and width as a function of wavevector \(q\). Eq.(5.7) is simply the large \(a\) limit of Eq.(5.4).

The unusual shapes of the resonances, which are evident in Fig. 5-1, can be understood by evaluating the quantity \(\delta G(\epsilon) = G(\epsilon) - G(\epsilon_0)\) that displays the dependence on \(\epsilon\) around the peak more clearly. Using Eq.(5.7) we write

\[
\delta G(\epsilon) = G_0 W \int \left(|tt(\epsilon, q)|^2 - |tt(\epsilon_0, q)|^2\right) dq. \tag{5.8}
\]

Since the difference of the two terms under the integral quickly goes to zero for \(\gamma(q) \gg |\epsilon - \epsilon_0|\), near the resonance, \(\epsilon \approx \epsilon_0\), the integral is dominated by small \(q\). Using quadratic model dependencies \(\epsilon_0(q) = \epsilon_0 + \alpha q^2\), \(\gamma(q) = \beta q^2\) which are valid at small \(q\), we can simplify the expression for \(\delta G\) as follows

\[
\delta G(\epsilon) = \frac{G_0 W \beta^{3/2}}{\beta^2 + \alpha^2} \int_{-\infty}^{\infty} du \frac{2\alpha \delta \epsilon u^2 - \delta \epsilon^2}{u^4 + (\delta \epsilon - \alpha u^2)^2}, \tag{5.9}
\]

with \(\delta \epsilon = \epsilon - \epsilon_0\), \(u = \sqrt{\beta}q\) and \(\tilde{\alpha} = \alpha / \beta\).

To evaluate this integral, we rewrite it using the primary fraction decomposition,

\[
\frac{2\tilde{\alpha} u^2 \delta \epsilon - \delta \epsilon^2}{u^4 + (\delta \epsilon - \tilde{\alpha} u^2)^2} = \frac{(\tilde{\alpha} + i) \delta \epsilon}{u^2 + i(\tilde{\alpha} u^2 - \delta \epsilon)} + \text{c.c.}. \tag{5.10}
\]

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Integration can be done using the formula
\[ \int_{-\infty}^{\infty} \frac{du}{au^2 + b} = \frac{\pi}{\sqrt{ab}}, \quad (5.11) \]
where for complex \( a \) and \( b \) the branch of the square root corresponding to positive real part of \( \sqrt{b/a} \) should be used. This gives
\[ \delta G(\epsilon) = -G_0 W \cos\left(\frac{3\phi}{2} + \frac{\pi}{4} \text{sgn}(\delta\epsilon)\right) \frac{|\delta\epsilon|}{(1 + \tilde{a}^2)^{3/2}} \sqrt{\frac{\beta}{\epsilon}}, \quad (5.12) \]
where \( \phi = \arctan(\tilde{a}) \), a relative measure of the rates at which the resonance moves and widens as a function of \( q \). This analysis predicts a square root singularity, \( \delta G(\epsilon) \propto \sqrt{|\delta\epsilon|} \), describing the dependence of conductance on energy (or gate voltage) in a sufficiently small region near the center of the peak, in which the quadratic dependencies \( \epsilon_+(q) = \epsilon_0 + a q^2 \), \( \gamma(q) = \beta q^2 \) constitute a valid approximation. The values \( \alpha \) and \( \beta \) are determined by the details of the potential \( U(x) \), leading to a few different possible line shapes.

The different types of behavior, illustrated in Fig. 5-2, can be understood as follows. In the limit \( \alpha \ll \beta \), the position of the resonance is approximately stationary, producing a symmetric line shape (since the transmission profile is symmetric). In this case, \( \delta G(\epsilon) \) is negative, forming a cusp at \( \epsilon = \epsilon_0 \) [Fig. 5-2(a)]. As \( \alpha \) increases, the contributions of transmission with different \( q \) values move to one side of the resonance, resulting in a conductance line shape that is asymmetric around \( \epsilon \). For a sufficiently rapid moving resonance, at the critical value \( \alpha_c = \beta / \sqrt{3} \), the leading term for \( \delta G(\epsilon) \) on one side of the resonance vanishes, giving a flattened behavior \( \delta G \) vs. \( \epsilon \) [Fig. 5-2(b)]. Increasing \( \alpha \) above \( \alpha_c \) changes the sign of \( \delta G(\epsilon) \) [Fig. 5-2(c)]. For \( \alpha \gg \beta \), the resonance position moves fast as a function of \( q \) resulting in \( G(\epsilon) \) being positive only on one side of the resonance [Fig. 5-2(d)].

To obtain a quantitative answer, we turn to numerical simulations by calculating plane wave transmission using the Hamiltonian Eq.(5.1) in a model potential \( U(x) = \frac{1}{2} m \omega^2 x^2 \), for \(|x| < \sqrt{8} \ell\), where \( \ell = \frac{\hbar}{\sqrt{2m} \omega} \) is the harmonic oscillator length. Since the (plane wave) dispersion relation outside the parabolic region is \( \epsilon = \frac{v_F^2 + q^2}{2m} + U_0 \), with \( U_0 = 4 \hbar \omega \) implied by the continuity of the potential at \(|x| = \sqrt{8} \ell\), arbitrarily high \( q \) are not allowed. The
Figure 5-2: Schematic for the conductance peak shape $G(\epsilon)$ for different values of the parameter $\alpha$ describing the dispersion of the quasibound state, $\epsilon_{q}(q) = \epsilon + \alpha q^{2}$, Eq.(5.12). Small $\alpha \ll \beta$ corresponds to a cusp with a square-root profile (a). For $\alpha$ near the critical value $\alpha_{c} = \beta / \sqrt{3}$ the peak flattens out on one side (b). For $\alpha > \alpha_{c}$, the peak transforms into a monotonic line shape (c), (d). The results for positive $\alpha$ (shown) and for negative $\alpha$ are related by symmetry $\delta \epsilon \rightarrow -\delta \epsilon$. 
Figure 5-3: The ballistic conductance for a parabolic barrier in BLG, $U(x) = \frac{1}{2}m\omega^2 x^2$ described in the text. Chirality-induced confined states manifest themselves as resonances positioned at $\epsilon = \hbar\omega(n + \frac{1}{2})$, with $n = 0, 1, 2, 3$ for a gapless system. Results for gap values $E_g = 0$, $2\hbar\omega$, and $4\hbar\omega$ are shown. As described by Eq.(5.12), $\delta G \propto -\sqrt{|\epsilon|}$ in the gapless case, but the profile is smeared for nonzero gap. (Inset) Zoom-in on the resonance at $\epsilon = \frac{5}{2}\hbar\omega$ showing the rounding of the conductance peak as $E_g$ increases.

allowed $q$ values are limited by $q\ell \leq \sqrt{\epsilon/\hbar\omega - 4}$ as seen in Fig. 5-4. The transmission amplitude through $U(x)$ is obtained for a range of parameters $q$ and $E_g$, and by the Landauer formula, the conductance is proportional to the integral of transmission over $q$. To find transmissions, we solve the differential equations, Eq.(5.5). Since BLG Hamiltonian supports coexisting evanescent and plane wave states, the procedure for this solution is notably more complicated than that of the non-relativistic Schroedinger equation. The construction of proper physical states on both sides of the barrier involves combining plane wave states with evanescent wave states. Hence, we need to solve the ODE, Eq.(5.5), two times for each $q$ and $E_g$, once with an outgoing plane wave as the initial condition, and then again with a decaying evanescent wave. The physical solution is the proper linear combination
of these two, such that the coefficient of the growing evanescent wave on the other side is zero. This process also provides the transmission coefficients readily. A full discussion of the methodology is given in Appendix C.

At zero gap, the numerical results confirm our analytic solution. The conductance in Fig. 5-3 and Fig. 5-1 show resonances approximately at energy levels of the bound states in the center regions, i.e. the harmonic oscillator energies: $\epsilon_n = (n + \frac{1}{2})\hbar\omega$, and $n = 0, 1, 2, \ldots$. The cusp in conductance is consistent with $\delta G(\epsilon) \propto \sqrt{\delta \epsilon}$.

Since the top and back gates used to create p-n-p junctions in BLG devices naturally create a potential difference between the two layers, it is crucial that we consider the effects of opening a gap [81, 2]. From the coupled equations Eq.(5.5), we see that for $E_g \neq 0$ and at $q = 0$, there is a coupling between the confined and deconfined states $\psi_+$ and $\psi_-$ of order $E_g$. This coupling limits the width of a resonance in transmission by $\gamma(q) \propto E_g^2$ when $q = 0$, which sets the minimum cusp width for conductance peaks to be of order $E_g^2$ (see Fig. 5-4). We also note that there is a line of transmission zeros away from $q = 0$, which corresponds to the situation where the right hand side of Eq.(5.5) is zero. If we approximate $(\frac{d}{dx})^{-1}$ as $\lambda = \frac{\hbar}{\sqrt{2m\epsilon}}$, we find a curve described by $q\ell = \frac{E_g\hbar^2}{4\sqrt{\epsilon}\hbar\omega}$, which shows that the transmission zero gets closer to $q = 0$ for increasing $\epsilon$. Also, the curve collapses to $q = 0$ when $E_g$ goes to zero, as expected from anti-Klein tunneling.

The gap is a function of the top and back gate voltages and can be continuously tuned to zero [40, 82]. In addition, the intrinsic gap from electron-electron interactions in the absence of a perpendicular electric field is estimated to be less than 1 meV [83]. We can compare this value to an estimated oscillator energy $\hbar\omega \approx 20$ meV for a real device, such as the one in Ref. [32]. Using the Thomas-Fermi approximation, $U(x) = \frac{h^2}{2m}\pi\rho(x)$, where $\rho(x)$ is the density and Taylor expanding the density in Ref. [32], we find the oscillator energy scale $\hbar\omega \approx 20$ meV for top gate voltages $\sim 3$ V. Thus, for a device where all three (p-n-p) regions can be independently gapped and gated, the decoupled states are clearly visible. Many currently available devices have one single back gate, and one local top gate. For these devices, we estimate that the gap size is typically much larger than the oscillator energy (See Appendix B).

To summarize, we predict a non-Lorentzian resonance line shape for the ballistic con-
ductance of BLG in a \textit{pnp} junction. The resonance shows a square root dependence on the energy/gate voltage that can generally be asymmetric around the resonance. The shape results from a vanishing coupling between bound and scattering states at normal incidence, and is a clear indication of chiral effects in a transport measurement.
Figure 5-4: Transmission and conductance of the gapless system (top), and gapped systems with $E_g = \hbar \omega$ (middle) and $E_g = 4\hbar \omega$ (bottom). Axis labels are the same as those in Fig. 5-1. The resonances correspond to the $E = \frac{1}{2} \hbar \omega, \frac{3}{2} \hbar \omega, \frac{5}{2} \hbar \omega$, and $\frac{7}{2} \hbar \omega$ harmonic oscillator bound states. As the gap $E_g$ increases, $E_g$ becomes the dominant resonant tunneling coupling, and the distinctive square root lineshape is cut off at small $\delta \epsilon$ by $E_g^2$. 
Chapter 6

Conclusion

Through the previous chapters, we have looked at a variety of interesting physical effects due to the unusually properties of monolayer and bilayer graphene. We have seen that both systems hold great potential for testing hitherto unseen physical effects. In this chapter, we summarize our results, and reiterate how the Dirac properties of monolayer graphene, and the massless chiral properties of bilayer graphene have allowed us access to these unusual effects. Finally, we reflect on the work that was done, and also give some viewpoints for the outlook in the field of charge transport in graphene.

6.1 Summary of Results

In Chapter 3 we used the Lorentz invariance of the effective monolayer graphene Hamiltonian to derive the ballistic contribution to magnetoconductance. By using the Lorentz symmetry, we were able to simplify the system of a monolayer in a p-n junction and a perpendicular magnetic field to a boosted system with only an electric field. The result was then confirmed with a semiclassical calculation. The form of the Hamiltonian will allow the techniques of Special Relativity to be applied in monolayer graphene.

Following our discussion of Dirac physics, we moved on to a monolayer system in a p-p'-p junction. We predicted and observed the collapse of Landau levels under the application of a deconfining potential. Here, the crucial physics was competition between the magnetic field and electric potential. The crossover regime relies on the cyclotron
radius and the potential variation length scale to be of the same magnitude. This collapse phenomenon can be seen in graphene as a direct result of our ability to create narrow local gates, which create potentials that vary on the order of 10 nm. Our ability to control the potential variation length scale can be used to probe other phenomena as we cross other length scales, such as the mean free path.

Finally, our last system involved bilayer graphene in a heterojunction. Here, we found that the unique band structure of bilayer graphene prevents crossing a p-n junction at normal incidence. This anti-Klein tunneling that a state can exist inside the potential that has vanishing coupling to outside extended states. The manifestation in transport was an unusual conductance line shape with a sharp peak. The introduction of a gap eliminates the orthogonality of the pseudospins on the p and n sides, and introduces a minimal width to the conductance peak.

6.2 Outlook

Much of the outlook for the work in this thesis can be found directly by looking at experimental efforts to probe the predicted effects. In the case of magnetoconductance in monolayer p-n junction, it was found that the ballistic limit is difficult to achieve [74, 75] and non-linear screening may dramatically affect the results [71]. Here we find two separate direction to consider. One is working towards better sample mobility to probe ballistic effects, towards which significant progress has already been made. The second direction is the inclusion of many body effects and disorder on our transport calculations.

By looking at our results on Landau level collapse, we can ask what happens in the case of bilayer graphene? The answer is that the collapse occurs at a fixed value of magnetic field for the case of a parabolic potential. The semiclassical analysis carries over into bilayer graphene as well. These are portions of unfinished work, not included in this thesis.

For a bilayer graphene in a p-n-p junction, we can think about subtleties that occur with the inclusion of different gaps in both the outer and middle regions. In real experimental devices, it is almost inevitable to create a gap in at least one of the regions. However, recently, multiple top gates with a single back gate has afforded some degree of independently
varying carrier density and gap. Another interesting possibility is to use a Fano resonance to create a non-monotonic I-V curve. Our calculations with the parabolic potential do not show such a conductance shape, but other potentials may, such as a square well.

What we have done here, in this thesis, traverses only a tiny region of the accumulated graphene literature. However, even in this small domain, we find a rich diversity of interesting effects. The world of graphene is young, and it is left to be seen what final impact it will have on the world. But, it is already clear that theorists and experimentalists alike have found a new playground, where we can answer old question, and pose new ones.
Appendix A

Landau level collapse, realistic potential

In the main text we modeled the behavior of the barrier potential induced by the top gate using an inverted parabola approximation $U(x) = -ax^2$. This form of the model potential was chosen because the spatial extent of the collapsing Landau level states is only a few magnetic lengths, which is smaller than the top gate width. Thus it was argued that the parabolic model is adequate for explaining experiments in top-gated structures. In addition, the parabolic model is convenient because semiclassical dynamics in this case can be easily treated analytically.

However, the parabolic potential increases indefinitely without bound for large $x$, raising concerns about possible unphysical behavior. To understand better the effects of barrier potential flattening outside the top-gated region, here we present numerical results for an asymptotically flat potential. These results confirm that the Landau level collapse behavior near the neutrality point only depends on the local curvature and is independent of the behavior of the potential as $|x| \rightarrow \infty$.

We use a Lorentzian potential to approximate the effects of the top and back gates.

$$U(x) = \frac{U_0}{1 + x^2/\ell^2} - \Delta U = U_0 \left( \frac{1}{1 + x^2/\ell^2} - 1 \right), \quad (A.1)$$

where we set $\Delta U = U_0$ to make the $pp'p-pnp$ crossover at the center of the top-gated region ($x = 0$) to occur at zero energy. The parameters $U_0$ and $\ell$ in our simulation can be matched to those in experiment by comparing Eq.(A.1) to the density profile found from
a finite element simulation of the experimental gate geometry [see A. F. Young & P. Kim, Nature Phys. 5, 222 (2009)],

$$e \rho(x) = \frac{C_{tg} V_{tg}}{1 + x^2/w^2} + C_{bg} V_{bg},$$  \hspace{1cm} (A.2)

where we restrict ourselves to the region of top gate voltages near neutrality, $C_{tg} V_{tg} + C_{bg} V_{bg} = 0$. Using the Thomas-Fermi approximation, we write the potential energy as a function of the local Fermi wavevector:

$$\epsilon - U(x) = \hbar v_F k_F(x),$$  \hspace{1cm} (A.3)

where $\epsilon$ is the Fermi energy. We then obtain the quantity

$$U_0 = \hbar v_F [k_F(0) - k_F(\infty)] = \hbar v_F \sqrt{\frac{\pi C_{bg} V_{bg}}{e}} \approx 0.25 \text{ eV},$$  \hspace{1cm} (A.4)

where $C_{bg} = 115 \frac{\text{eV}}{\mu m^2}$, $V_{bg} = -70 \text{ V}$. We also take the width of the potential in Eq.(A.1) to be equal to the width of the Lorentzian density profile, $\ell = w = 50 \text{ nm}$.

Using these parameters, we define the energy scale, length scale, and magnetic field scale in terms of the curvature of the potential $U(x)$ at small $x$: $U(x) \approx a x^2$, $a = \frac{U_0}{\ell^2}$. This gives

$$\epsilon_* = (\hbar^2 v_F^2 a)^{1/3}, \quad x_* = \left(\frac{\hbar v_F}{a}\right)^{1/3}, \quad B_* = \frac{\hbar}{e} \left(\frac{a}{\hbar v_F}\right)^{2/3}.$$  \hspace{1cm} (A.5)

Converting the magnetic field scale $B_*$ to real units we find

$$B_* = \frac{\hbar}{e} \left(\frac{U_0}{\ell^2 \hbar v_F}\right)^{2/3} = 1.9 \text{ T},$$  \hspace{1cm} (A.6)

which sets the scale for the region where Landau level collapse occurs.

The results of the simulation with the potential (A.1) are shown in Fig. A-1. The behavior is essentially the same as in the parabolic case with some deviations seen far from neutrality in the $pp'p$ regime (large negative $\epsilon$). The observed deviation can be understood semiclassically, since classical orbits with larger total energy $\epsilon$ have greater spatial extent and thus can feel the long range part of the potential $U(x)$. In contrast, the orbits with
small $\epsilon$ are confined to the region where the parabolic model is accurate. We also note that using the experimental parameters, we obtain an estimate of critical field $B_c \sim 5$ T which compares well with experiment.

Figure A-1: Density of electronic states for the Lorentzian model of the barrier potential, Eq.(A.1). Shown is the derivative of the density of states at the center of the top-gated region with respect to energy, $\frac{dN}{d\epsilon}$. The simulation was conducted in the same way as described in the main text, using system size $L = 20x_*$, energy level broadening $\Gamma = 0.1\epsilon_*$, and $M = 1500$ points of spatial discretization. The dashed parabola $B_c(\epsilon) = \pm(2/3v_F) \sqrt{-ae}$ marks the critical field in the parabolic model, $U(x) = -ax^2$. 
Appendix B

Chirality-assisted confinement, gap estimation

In this appendix, we consider a realistic situation using the device in Ref. [32] as an example. We will analyze the middle region of a p-n-p junction in the presence of both top and back gates. In this case, the differences in electrostatic potential generates an unscreened gap $E_g^0$ between the BLG layers. However, due to the non-zero density of states at low energies, the gap is heavily screened. The effective gap can be approximated as [38, 84]

$$E_g(n) = \frac{E_g^0 + \gamma_1 n/n_0}{\Lambda^{-1} + |n/n_0| - \frac{1}{2} \log |n/n_0|},$$  \hspace{1cm} (B.1)

where $E_g^0$ is the unscreened gap, $n$ is the carrier density, $n_0 = \frac{\gamma_1^2}{\pi \hbar^2 v_F} \approx 1.18 \times 10^{13}$/cm$^2$, and $\gamma_1 = 0.4$ meV. The parameter $\Lambda^{-1} = \frac{2\pi \hbar^2 v_F^2 c_0}{e^2 \gamma_1 c_0} \approx 1$ measures the intrinsic screening effectiveness of BLG, where $c_0 = 3.35$ Å is the interlayer spacing and $\varepsilon_r \approx 1$ is the (relative) dielectric constant of BLG. Using the known values, including $v_F = 1 \times 10^6$ m/s, we find $\Lambda^{-1} = 1.12\varepsilon_r$. This formula is only to be used for intermediate densities, $|E_g^0| \ll |\varepsilon_F| < \gamma_1$.

The carrier density is determined by the capacitive coupling to the gates

$$n = \frac{1}{e} (C_b V_b + C_t V_t),$$  \hspace{1cm} (B.2)

where $e$ is the electron charge, $C_(t(b))$ is the capacitance per unit area of the top (back) gate,
and \( V_{t(b)} \) is the top (back) gate voltage away from charge neutrality.

BLG experiences an electric displacement equal to the average of the displacement fields from the top and bottom gates

\[
E_g^0 = \varepsilon_0 D = \frac{\varepsilon_0 \varepsilon_b}{2d_b} \left( V_b - \frac{C_t}{C_b} V_t \right),
\]

where \( d_{t(b)} \) is the distance to the top (back) gate, \( V_{t(b)} \) is the voltage away from charge neutrality. We have set \( V_b = 0 \) and \( V_t = 0 \) as the charge neutrality point.

For the device in Ref. [32], \( C_b = 116 \text{ aF/\mu m}^2 \), \( C_t = 1490 \text{ aF/\mu m}^2 \), \( \varepsilon_b = 3.9 \) (silicon), and \( d_b = 290 \text{ nm} \). Using \( \Lambda = 1 \), we plot the screened gap as a function of \( V_t \) and \( V_b \) Fig. B-1.

![Figure B-1: The screened gap \( E_g(n) \) as a function of top (\( V_t \)) gate and back gate (\( V_b \)) voltages. The black lines indicate \( n = \pm 10^{12}/\text{cm}^2 \), the blue lines \( n = \pm 5 \times 10^{11}/\text{cm}^2 \), and the white lines \( n = \pm 10^{11}/\text{cm}^2 \).](image)

The oscillator energy scale can be obtained from the density profile from the supplementary material of Ref. [32]. The charge density is

\[
\rho(x) = \frac{C_t V_t}{1 + |x/w|^2} + C_b V_b,
\]

where \( w = 50 \text{ nm} \). In the Thomas-Fermi approximation \( U(x) = \frac{\hbar^2}{2m} \pi \rho(x) \) the potential has
the quadratic contribution

\[ \frac{d^2 U(x)}{dx^2} \bigg|_{x=0} = -\frac{\hbar^2}{2m^*} \frac{C_i V_i}{\epsilon w^2}. \]  

(B.5)

Thus, the oscillator frequency is

\[ \hbar \omega = \hbar \sqrt{\frac{\hbar^2}{m^*}} \frac{C_i V_i}{\epsilon w^2} \approx 6.5 \text{ meV} \sqrt{V_i/(\text{Volt})}. \]  

(B.6)

Comparing the oscillator energy scale with the screened gap gives a picture of the dominant effect. For this device, the gap is always much larger than the oscillator energy. As a result, normal Lorentzian resonances are anticipated here.

Figure B-2: The oscillator energy scale divided by the gap \( \hbar \omega / E_g \) as a function gate voltages. In this system the oscillator energy is much smaller than the gap size. The black lines indicate \( n = \pm 10^{12} / \text{cm}^2 \), the blue lines \( n = \pm 5 \times 10^{11} / \text{cm}^2 \), and the red lines \( n = \pm 10^{11} / \text{cm}^2 \).

Another useful metric is the Fermi energy over the oscillator energy, which gives the number of resonances under the barrier. The Fermi energy is simply

\[ \epsilon_F = \text{sgn}(n) \sqrt{\left( \frac{\hbar^2}{2m^*} \pi n \right)^2 + \left( \frac{E_g^0}{2} \right)^2}. \]  

(B.7)

Dividing the Fermi energy by the oscillator energy shows for that for a p-n-p configuration with densities \( \sim 10^{12} / \text{cm}^2 \), there are \( \sim 7 \) resonances under the barrier.

Since the confined states are only well defined for \( E_g \ll \hbar \omega < \epsilon_F \), we must consider
Figure B-3: The Fermi energy divided by the oscillator energy approximates the number of resonances. The black lines indicate $n = \pm 10^{12}/\text{cm}^2$, the blue lines $n = \pm 5 \times 10^{11}/\text{cm}^2$, and the red lines $n = \pm 10^{11}/\text{cm}^2$.

devices with different parameters to realize the non-Lorentzian conductance lineshape. A simple modification is to decrease the width of the top gate potential. A smaller gate width $w$ will increase $\hbar \omega$. Another approach is to use suspended BLG, so that the lower capacitive coupling decreases the gap relative to the oscillator energy, $\hbar \omega/E_g \sim (C_i)^{-1/2}$ (at $V_b = 0$). A more difficult solution involves fabricating both top and bottom split gates, which will allow independent control of both gap and density in each region.
Appendix C

Chirality-assisted confinement, numerical procedure

In this appendix, we describe the procedure used in Chapter 5 to calculate transmission.

C.1 Overview

We assume the eigenstates are plane waves outside of the region of interest and evolve the wavefunction through the region of interest using an ordinary differential equation (ODE) solver.

The bilayer graphene Hamiltonian supports evanescent modes, and the transmission problem must be solved with the condition that no exponentially growing modes (in their respective directions) exist on either side. We find the physical solution by first giving a pure transmitted wave as an initial condition, and evolving the wavefunction through the junction. We then give a purely decaying wave as the initial condition and evolve again (Fig. C-1). The physical state is the linear combination where $B_1 = -B_2$.

C.2 Equation of evolution

In this section, we derive the equation that governs evolution inside the junction. We recast the problem in terms of a first order ODE, so that the first order ODE solver can be used.
Figure C-1: The physical transmission problem is the linear combination of these two situations where \( B_1 = -B_2 \).

We begin with the bilayer graphene Hamiltonian in a potential \( U(x) \) that only varies in the \( x \) direction. The wavevector \( k_y \) is conserved. We also include a gap \( \Delta \) and a perpendicular magnetic field \( B \). \( \hbar \) is set to 1.

\[
H = \begin{pmatrix}
U(x) + \Delta & \frac{1}{2m}(-i\partial_x - i(k_y - Bx))^2 \\
\frac{1}{2m}(-i\partial_x + i(k_y - Bx))^2 & U(x) - \Delta
\end{pmatrix}, \quad H\Psi = E\Psi, \quad \Psi = \begin{pmatrix}
\psi_1 \\
\psi_2
\end{pmatrix}.
\]

After rearrangement, we find two coupled second-order differential equations

\[
\begin{align*}
(E - U(x) - \Delta)\psi_1 &= -2m(\partial_x + k_y - Bx)^2\psi_2, \\
(E - U(x) + \Delta)\psi_2 &= -2m(\partial_x - k_y + Bx)^2\psi_1.
\end{align*}
\]

In order to obtain a 4-component, first-order differential equation, we define the gauge derivatives \( \phi_1 \) and \( \phi_2 \),

\[
\begin{align*}
\phi_1 &= (\partial_x + k_y - Bx)\psi_2, \\
\phi_2 &= (\partial_x - k_y + Bx)\psi_1, \\
-2m(E - U(x) - \Delta)\psi_1 &= (\partial_x + k_y - Bx)\phi_1, \\
-2m(E - U(x) + \Delta)\psi_2 &= (\partial_x - k_y + Bx)\phi_2,
\end{align*}
\]

which yields

\[
\partial_x \begin{pmatrix}
\phi_1 \\
\psi_1 \\
\phi_2 \\
\psi_2
\end{pmatrix} = \begin{pmatrix}
Bx - k_y & -2m(E - U(x) - \Delta) & 0 & 0 \\
0 & k_y - Bx & 1 & 0 \\
0 & 0 & k_y - Bx & -2m(E - U(x) + \Delta) \\
1 & 0 & 0 & Bx - k_y
\end{pmatrix} \begin{pmatrix}
\phi_1 \\
\psi_1 \\
\phi_2 \\
\psi_2
\end{pmatrix}.
\]
C.3 Connecting to plane waves

In this section we will derive the appropriate input and output wavefunctions in terms of plane waves and evanescent waves.

Our wavefunctions at each end are assumed to be the asymptotic solutions of BLG in the absence of any potential, gap, or magnetic field. In this case, the Hamiltonian is simply

$$H = \frac{1}{2m} \begin{pmatrix} 0 & (\hat{p}_x - i\hat{p}_y)^2 \\ (\hat{p}_x + i\hat{p}_y)^2 & 0 \end{pmatrix}, \quad H\Psi = E\Psi, \quad \Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}. \quad (C.5)$$

This simple system yields eigenvalues $E_{\pm} = \pm \epsilon \equiv \pm (k_x^2 + k_y^2)/2m$, where $k_x$ and $k_y$ are the momentum eigenvalues in the $x$ and $y$ directions. The eigenvectors of $H$ can be found via

$$(H - E_{\pm})\Psi = 0 \quad \rightarrow \quad \psi_1 = \pm \frac{(k_x - i k_y)^2}{\epsilon} \psi_2 = \pm e^{-2i\theta} \psi_2. \quad (C.6)$$

For simplicity and definiteness, we restrict ourselves to positive energies ($E_+$). The normalized plane wave solutions are

$$\psi^+ = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i2\theta} \\ 1 \end{pmatrix} e^{ik_x x + ik_y y}, \quad \psi^- = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i2\theta} \\ 1 \end{pmatrix} e^{-ik_x x + ik_y y}. \quad (C.7)$$

Under a substitution $k_x = i\kappa$, we can find the (unnormalized) evanescent solutions

$$\psi^A = \begin{pmatrix} -(\kappa - k_y)^2 \\ k_x^2 - k_y^2 \end{pmatrix} e^{-\kappa x + ik_y y}, \quad \psi^B = \begin{pmatrix} (\kappa + k_y)^2 \\ k_x^2 - k_y^2 \end{pmatrix} e^{\kappa x + ik_y y}. \quad (C.8)$$

The value of $\kappa$ is free, so in the simulations we choose $\kappa = 0$ for simplicity.
C.3.1 Initial conditions

Using the wavefunction for a left moving plane wave, $\psi^-$, our initial condition for one run is

$$
\begin{pmatrix}
\phi_1 \\
\psi_1 \\
\phi_2 \\
\psi_2
\end{pmatrix} =
\begin{pmatrix}
-ik_x + k_y - Bx \\
e^{2i\theta} \\
(-ik_x - k_y + Bx)e^{2i\theta} \\
1
\end{pmatrix}
\begin{pmatrix}
e^{-ik_x+k_y} \\
e^{-ik_x+k_y} \\
e^{i(kx+ky)} \\
\frac{1}{\sqrt{2}}
\end{pmatrix},
\qquad x = -L \text{ (left boundary)}. 

(C.9)

The other run uses the evanescent wavefunction, $\psi^+$, so the initial condition is

$$
\begin{pmatrix}
\phi_1 \\
\psi_1 \\
\phi_2 \\
\psi_2
\end{pmatrix} =
\begin{pmatrix}
\kappa + k_y - Bx \\
\left(-\frac{(k+k_y)^2}{-\kappa^2+k_y^2}\right) \\
-(\kappa - k_y + Bx)\left(\frac{(k+k_y)^2}{-\kappa^2+k_y^2}\right) \\
1
\end{pmatrix}
\begin{pmatrix}
\kappa e^{ikx+k_y} \\
\kappa e^{ikx+k_y} \\
e^{-\kappa x} \\
1
\end{pmatrix},
\qquad x = -L \text{ (left boundary)}. 

(C.10)

C.3.2 Final conditions

The output from the ODE solver will be a linear superposition of the traveling and evanescent waves

$$
\psi_{\text{out}} = \frac{1}{t} \psi^- + \frac{r}{t} \psi^+ + A\psi^A + B\psi^B. 

(C.11)

To unscramble them, we need a matrix $M$

$$
\begin{pmatrix}
\phi_1 \\
\psi_1 \\
\phi_2 \\
\psi_2
\end{pmatrix} =
\begin{pmatrix}
\frac{1}{t}e^{-ik_x} \\
\frac{\xi e^{ik_x}}{t} \\
\frac{\zeta e^{ik_x}}{t} \\
\Lambda e^{-\kappa x} \\
Be^{\kappa x}
\end{pmatrix},
\qquad (C.12)\)
where the matrix $M$ is

\[
\begin{pmatrix}
(-ik_x + k_y - Bx) & (ik_x + k_y - Bx) & (-\kappa + k_y - Bx) & (\kappa + k_y - Bx) \\
e^{2i\theta} & e^{-2i\theta} & \frac{(\kappa - k_y)^2}{k_f^2 - \kappa^2} & \frac{(\kappa + k_y)^2}{-k^2 + k_f^2} \\
(-ik_x - k_y + Bx)e^{2i\theta} & (ik_x - k_y + Bx)e^{-2i\theta} & -\frac{(\kappa - k_y)^2}{k_f^2 - \kappa^2}(-\kappa - k_y + Bx) & -\frac{(\kappa + k_y)^2}{-k^2 + k_f^2}(\kappa - k_y + Bx) \\
1 & 1 & 1 & 1
\end{pmatrix},
\]

and $x = L$ is evaluated at the right boundary. The inverse of this matrix is used to find the transmission and reflection coefficients.
Bibliography


