# Quantum Oscillations in Twisted Bilayer Graphene 

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## Contents

Introduction ..... 5
1 Models ..... 7
1.1 Graphene ..... 7
1.1.1 Lattice Properties ..... 7
1.1.2 Band Structure ..... 8
1.2 Twisted Bilayer Graphene ..... 9
1.2.1 Lattice Properties ..... 10
1.2.2 Band Structure ..... 11
2 Quantum Oscillations ..... 15
2.1 Electrons in a Magnetic Field ..... 15
2.2 Quantization of Orbits in a Magnetic Field ..... 16
2.3 De Haas-Van Alphen Effect ..... 17
2.4 Example with Graphene ..... 17
2.5 Twisted Bilayer Graphene ..... 18
3 Numerical Method ..... 19
3.1 Quantization Using Ladder Operators ..... 19
3.2 Numerical Implementation of Ladder Operators ..... 20
3.2.1 Example with Graphene ..... 21
3.2.2 Difficulty in Obtaining Landau Levels Analytically for TBG ..... 21
3.2.3 Numerical Computation of TBG Landau Levels ..... 22
4 Lifshitz-Kosevich Formula ..... 25
4.1 General Case ..... 25
4.2 Graphene ..... 26
4.2.1 Specific Heat ..... 30
4.3 Twisted Bilayer Graphene ..... 30
5 Results ..... 33
5.1 Method ..... 33
5.2 Results for Graphene ..... 34
5.3 Results for Twisted Bilayer Graphene ..... 34
Conclusion and Outlook ..... 396 Appendicies41
6.1 Appendix A: Poisson Summation ..... 41

## Introduction

In his 1930 paper[15], physicist Lev Landau applied quantum mechanical rules to electrons in a magnetic field to show that they describe quantized orbits. In other words, charged particles in classical mechanics describe orbits when placed in a magnetic field, but when quantum mechanics is considered, such particles are restricted to certain orbits. Landau then suggested that the magnetization should oscillate as the magnetic field is increased, but claimed such an effect could not be observed experimentally due to lack of proper technology. He was proved wrong only a month later, when De Haas and Van Alphen discovered the effect in Bismuth crystal[9]. It turned out that Bismuth had a particular structure which allowed for the de Haas-van Alphen (dHvA) effect, as it was so named, to be easily observed.

The following years did not yield further understanding of the phenomena, but a breakthrough appeared when in 1947 J. A. Marcus[21] observed the dHvA effect in zinc. This showed that Bismuth was not unique in this respect, which was contrary to the consensus at the time. By 1952, 13 metals had been investigated, and only one of them did not show oscillatory behaviour. Around the same time, Onsager[25] derived a relation between the frequency of oscillation, and the cross-sectional area of the Fermi surface, which provided a tool to investigate the Fermi surface of metals. Similarly, Lifshitz and Kosevich[16], who had developed the same idea on their own, published a detailed theory of the dHvA effect which determined the frequency and amplitude.

By the 1960 's, most metals showed the dHvA effect, and as superconducting magnets entered laboratories, the precision of measurement greatly improved. After an important conference in New-York, many other methods were used to determine the Fermi surface, although the dHvA effect remained the most versatile and accurate. Furthermore, oscillations in other properties were also found, such as oscillations in the electrical resistance, which is referred to as the Shubnikovde Haas ( SdH ) effect. Nevertheless, the underlying cause of all such oscillations is the same, and together, they are referred to as quantum oscillations. Today, quantum oscillations are still widely used as a tool to probe the Fermi surface of metals, where they are used for example to investigate conventional superconductors[8].

In 2004, graphene, a 2-dimensional carbon structure, was first identified in laboratory[24]. This discovery was widely acclaimed, since graphene was expected to have very interesting properties, such as high electrical and thermal conductivity. At the same time, superpositions of several graphene layers were also observed, among which was twisted bilayer graphene (TBG), a superposition of two graphene sheets characterized by a relative twist angle. In 2011, it was theoretically shown that at specific angles, also called magic-angles, TBG demonstrated superconductive behaviour[2], and in 2018, this was demonstrated experimentally $[5,6]$. In any case, quantum oscillations were an important part of experimental research, providing information on electron transport and the Fermi surface of both graphene and TBG.

The objective of this thesis is to obtain an analytical derivation of quantum oscillations in TBG, and to compare it to numerical calculations. The first chapter will introduce the models used
in this thesis, namely graphene and TBG, where graphene will be used as a testing model. The second chapter introduces quantum oscillations, where the relevant theory will be covered and then applied to graphene and TBG. In the third chapter, the numerical method used in this thesis will be introduced, and will be used to make an analytical approximation for TBG. This analytical approximation will be used in the fourth chapter to obtain the quantum oscillations analytically. Finally, the full numerical results will be presented in the fifth chapter, and will be compared to the analytical results.

## Chapter 1

## Models

In this chapter, we introduce models relevant to this thesis. We first give an overview of graphene, which is used as a means to test concepts throughout this text, and then move on to the main model of this thesis, which is twisted bilayer graphene (TBG). For both systems, we introduce their properties and present the band structure. The section on graphene is based on mostly on refs. [7, 14], while the section on TBG is based on refs. [27, 10].

### 1.1 Graphene

Graphene[23] is a 2-dimensional material composed of carbon atoms arranged in a hexagonal honeycomb lattice, as illustrated in fig. 1.1(a). It is the starting point for various other carbon structures, such as fullerenes (balls of graphene) or nanotubes (rolled up graphene sheets), but more importantly, graphene can also be stacked up to form graphite, and it is in such arrangement that it appears naturally.

Although the existence of graphene as a single layer of graphite was theorized already in the 1920 's[1], it was believed that due to thermal effects, graphene would collapse onto itself if isolated. Nevertheless, in 2004, Geim and Novoselov[24] successfully extracted sheets of graphene from graphite using scotch tape. This largely impacted the research community, and for this reason they were awarded the Nobel Prize in 2010.

Following this discovery, it was discovered that graphene has a long list of remarkable properties[11, 33], such as high carrier mobility, breaking strength and thermal conductivity, as well as being impermeable to gases despite its thinness. As a result, graphene is the conversation piece for many potential applications[11, 26] in computer electronics, data storage, composite materials and electrical batteries, to cite only a few examples.

### 1.1.1 Lattice Properties

The honeycomb structure of graphene is illustrated in fig. 1.1(a). The sites A and B both represent identical Carbon atoms, but because their nearest neighbours are different, they must be distinguished as two different sub-lattices. For a site A, its nearest neighbours are located at

$$
\boldsymbol{\delta}_{1}=a(1,0), \quad \boldsymbol{\delta}_{2}=\frac{a}{2}(-1,-\sqrt{3}) \quad \text { and } \quad \boldsymbol{\delta}_{3}=\frac{a}{2}(-1, \sqrt{3},)
$$



Figure 1.1: a.) Graphene honeycomb structure with carbon atoms located on sites $A$ and $B$, lattice vectors $\boldsymbol{a}_{1}$ and $\boldsymbol{a}_{2}$, nearest neighbours for a site $A \boldsymbol{\delta}_{1}, \boldsymbol{\delta}_{2}$ and $\boldsymbol{\delta}_{3}$, and the dashed shape represents the unit cell. b.) First $B Z$ of graphene, with reciprocal lattice vectors $\boldsymbol{b}_{1}$, and $\boldsymbol{b}_{2}$, and special points $\Gamma, M, K$ and $K^{\prime}$. c.) Band structure of graphene for nearest neighbours, where the dashed shape represents the first BZ of graphene and the inset is a magnification of the spectrum around a corner of the BZ.
where $a \approx 0.142 \mathrm{~nm}$ is the carbon-carbon distance (and $\sqrt{3} a=a_{0}$, where $a_{0} \approx 0.246 \mathrm{~nm}$ is the lattice constant). Furthermore, the unit cell includes both a B site and an A site, and is illustrated in fig. 1.1(a) as a dashed line, and where the lattice vectors are

$$
\boldsymbol{a}_{1}=\frac{a}{2}(3, \sqrt{3}) \quad \text { and } \quad \boldsymbol{a}_{2}=\frac{a}{2}(3,-\sqrt{3}) .
$$

The first Brillouin zone (BZ) of the reciprocal lattice is shown in fig. 1.1(b), where

$$
\boldsymbol{b}_{1}=\frac{2 \pi}{3 a}(1, \sqrt{3}) \quad \text { and } \quad \boldsymbol{b}_{2}=\frac{2 \pi}{3 a}(1,-\sqrt{3})
$$

are the reciprocal lattice vectors. Note that the BZ has a hexagonal shape, which is chosen from convention. The first BZ of graphene features the special points $\Gamma$ at the centre, $M$ on the edges, and $K$ and $K^{\prime}$ on the corners, as shown in fig. 1.1(b). The $K$ and $K^{\prime}$ points are of significance, as will be shown in the following subsection, and are located at

$$
K=\left(\frac{2 \pi}{3 a}, \frac{2 \pi}{3 \sqrt{3} a}\right) \quad \text { and } \quad K^{\prime}=\left(\frac{2 \pi}{3 a},-\frac{2 \pi}{3 \sqrt{3} a}\right)
$$

where the remaining four corners can be obtained by a lattice translation. Note that $K^{\prime}=-K$

### 1.1.2 Band Structure

Each carbon atom has 6 electrons. Two of them fill the 1s state and have a negligible effect on the electronic properties. Three other electrons make up $3 \sigma$ bonds with all 3 of their neighbours, while the last electron make a $\pi$ bond with one other carbon atom. Since the $\pi$ bond is the weakest bond, it will be the most significant contributor to the electronic properties of graphene.

In second quantization, we define the annihilation (creation) operator $\hat{a}_{\sigma, i}\left(\hat{a^{\dagger}}{ }_{\sigma, i}\right)$ for a $\pi$-bond electron situated at site $i$ on the sub-lattice A with spin $\sigma$, and a similar definition holds for the operators $\hat{b}$ on sub-lattice B. The energy spectrum of the electrons is described by assuming that electrons can hop to nearest and next-nearest sites, and the resulting tight-binding Hamiltonian is

$$
\begin{equation*}
H=-t \sum_{\langle i, j\rangle, \sigma}\left(\hat{a}_{\sigma, i}^{\dagger} \hat{b}_{\sigma, j}+\text { h.c. }\right)-t^{\prime} \sum_{\langle\langle i, j\rangle\rangle, \sigma}\left(\hat{a}_{\sigma, i}^{\dagger} \hat{a}_{\sigma, j}+\hat{b}_{\sigma, i}^{\dagger} \hat{b}_{\sigma, j}+\text { h.c. }\right), \tag{1.1}
\end{equation*}
$$

where $t(\approx 2.8 \mathrm{eV})$ and $t^{\prime}(0.02-0.2 \mathrm{eV})$ are the nearest and next-nearest hopping parameters determined by experiments. This Hamiltonian was first diagonalized by Wallace[35] in 1947, and the resulting eigenvalues are

$$
\begin{equation*}
\epsilon_{ \pm}(\boldsymbol{k})= \pm t \sqrt{3+f(\boldsymbol{k})}-t^{\prime} f(\boldsymbol{k}) \tag{1.2}
\end{equation*}
$$

with

$$
f(\boldsymbol{k})=2 \cos \left(\sqrt{3} k_{y} a\right)+4 \cos \left(\frac{\sqrt{2}}{2} k_{y} a\right) \cos \left(\frac{3}{2} k_{x} a\right)
$$

The ' + ' sign in eq. 1.2 refers to the conduction band (the upper band) and the ' - ' sign refers to the valence band (the lower band). The spectrum is shown in fig. 1.1(c) for $t^{\prime}=0$, and in the case where $t^{\prime} \neq 0$, the conduction and valence bands are asymmetric.

Since every carbon atom contributes 1 electron to a $\pi$ bond, and since each electron can occupy a spin up or spin down state, the valence band will be completely filled, while the conduction band will be empty. This means that any small excitation will occur around the point where the bands touch, which happens at zero energy for the case where $t^{\prime}=0$. Furthermore, from eq. 1.2, we can see that $\epsilon_{ \pm}(\boldsymbol{k})=\epsilon_{ \pm}(-\boldsymbol{k})$ and therefore any $\boldsymbol{k}$ satisfying $\epsilon_{ \pm}(\boldsymbol{k})=0$ is paired with an equivalent $-\boldsymbol{k}$ that satisfies $\epsilon_{ \pm}(-\boldsymbol{k})=0$. It happens that such pairs of solutions are located at the two in-equivalent corners $K$ and $K^{\prime}$, which are indeed related by $K^{\prime}=-K$, as seen in fig. 1.1(b).

By expanding the spectrum around such points, we get Dirac equations for massless fermions

$$
\begin{equation*}
h^{K}(\boldsymbol{k})=v_{F} \boldsymbol{\sigma} \cdot \boldsymbol{k} \quad \text { and } \quad h^{K^{\prime}}(\boldsymbol{k})=v_{F} \boldsymbol{\sigma}^{*} \cdot \boldsymbol{k} \tag{1.3}
\end{equation*}
$$

for the $K$ and $K^{\prime}$ points respectively, where the speed of light $c$ is replaced by the Fermi velocity $v_{F}=3 t a / 2\left(\approx 10^{6} \mathrm{~ms}^{-1}\right)$, and $\boldsymbol{\sigma}=\left(\sigma^{x}, \sigma^{y}\right)$. In this context, the Pauli matrices $\sigma^{x}$ and $\sigma^{y}$ do not refer to real spin, but rather to a pseudo-spin associated with the two sub-lattices. Also note that the momentum $\boldsymbol{k}$ is now relative to the $K$ or $K^{\prime}$ points, which are also called Dirac points due to the emergence of the Dirac equation. The eigenvalues of eq. 1.3 are

$$
\begin{equation*}
\epsilon_{ \pm}(\boldsymbol{k})= \pm v_{F}|\boldsymbol{k}|, \tag{1.4}
\end{equation*}
$$

which represent a so-called Dirac cone as seen in the inset of fig. 1.1(c), and are identical for both the $K$ and $K^{\prime}$. The emergence of Dirac equations for low energy has many interesting consequences, such as states with a well defined chirality, which is broken at higher energies. Furthermore, since the Dirac points come in pairs, the energy levels are doubly degenerate.

### 1.2 Twisted Bilayer Graphene

Twisted bilayer graphene (TBG) is a material composed of two superimposed graphene sheets with a relative twist angle, as see in fig. 1.2(a). Due to the relative angle, the two honeycomb patterns of the underlying graphene sheets interfere visually with each other to produce an array of light and dark regions. The resulting interference is called a Moiré pattern, and it was believed that such pattern could drastically modify the physics of the system[18].

As a matter of fact, in 2011, Bistritzer and MacDonald[2] were able to demonstrate numerically that at specific angles, called magic angles, TBG becomes superconductive. This discovery was later confirmed by experiments $[5,6]$ done at $1.05^{\circ}$, the highest magic angle, where superconductivity was observed for temperatures of 1.7 K . This has attracted a lot of attention, mainly due to the ability to easily tune the onset of superconductivity with a magnetic field.

In contrast to conventional superconductors, for which the relevant theory is 50 years old, TBG is considered an unconventional superconductor and lacks proper theoretical understanding. For this reason, considerable interest remains in studying TBG at magic angles[20], despite it having few real-world applications as a superconductor, due to the high sensitivity of the superconductive state with twist angle.

### 1.2.1 Lattice Properties

As a consequence of the relative twist angle $\theta$, the hexagonal pattern of the two superimposed graphene layers interfere with each other to produce Moiré patterns. The result is the appearance of lighter areas that are periodic is space and separated by darker regions, as can be seen in fig. 1.2(a). In the case of twisted bilayer graphene (TBG), the Moiré pattern is hexagonal, with period (i.e. the distance between light areas)

$$
\begin{equation*}
L_{\text {Moiré }}=\frac{\sqrt{3} a}{2 \sin (|\theta| / 2)} \tag{1.5}
\end{equation*}
$$

where $a \approx 0.142 \mathrm{~nm}$ is again the carbon-carbon distance, and the equation is valid only for $|\theta|<\pi / 6$. Since a hexagon is symmetric under a $\pi / 3$ rotation, angles larger than $\pi / 3$ can be reached using $\theta^{\prime}=\pi / 3-\theta$ in eq. 1.5. Hence, the Moiré period decreases as the angle increases up until $\theta=\pi / 6$, after which it increases back again only to diverge at $\theta=\pi / 3=0$.

While the Moiré pattern exists for any angle, the actual structure of TBG is not necessarily periodic. This is significant, because the absence of periodicity prohibits from using tight binding to obtain the band structure, which drastically complicates the issue. In the case when the twisted graphene sheets do indeed give rise to a periodic superstructure, we say that the structure is commensurable, and we can define the lattice vectors

$$
\boldsymbol{L}_{1}=n \boldsymbol{a}_{1}+m \boldsymbol{a}_{2}=n^{\prime} \boldsymbol{a}_{1}^{\prime}+m^{\prime} \boldsymbol{a}_{2}^{\prime}
$$

and $\boldsymbol{L}_{2}=R(\pi / 3) \boldsymbol{L}_{1}$, where $R(\theta)$ is the 2 d rotation matrix, $\boldsymbol{a}_{(1,2)}$ are the graphene lattice vectors, $\boldsymbol{a}_{(1,2)}^{\prime}=R(\theta) \boldsymbol{a}_{(1,2)}$ with $\theta$ the twist angle, and $n, m, n^{\prime}$ and $m^{\prime}$ are integers. Hence, the condition for the superstructure to be periodic is to enforce $n \boldsymbol{a}_{1}+m \boldsymbol{a}_{2}=n^{\prime} \boldsymbol{a}_{1}^{\prime}+m^{\prime} \boldsymbol{a}_{2}^{\prime}$. The solutions to this equation are not obvious, and are discussed in [29, 30]. In any case, the resulting requirement on the twist angle $\theta$ is[10]

$$
\begin{equation*}
\cos (\theta)=\frac{3 q^{2}+3 q p+p^{2} / 2}{3 q^{2}+3 q p+p^{2}} \tag{1.6}
\end{equation*}
$$

where $q$ and $p$ are integers such that $\operatorname{gcd}(q, p)=1$, with gcd the greatest common denominator, and $\pi / 3>\theta>0$. The limit $p \ll q$ corresponds to $\theta=0$ while the limit $p \gg q$ to $\theta=\pi / 3$. Commensurable angles that lie outside the specified range are obtained by considering the geometrical symmetries of graphene mentioned above. The set of possible values for $(q, p)$ can be classified by whether $\operatorname{gcd}(p, 3)=1$ or $\operatorname{gcd}(p, 3)=3$. These two different sets of solutions amount to details that are out of the scope of this text, and for simplicity, we will stick to the case $\operatorname{gcd}(p, 3)=1$. Hence, for $\operatorname{gcd}(p, 3)=1$, the TBG lattice vectors can be expressed as

$$
\boldsymbol{L}_{1}=q \boldsymbol{a}_{1}+(q+p) \boldsymbol{a}_{2} \quad \text { and } \quad \boldsymbol{L}_{2}=-(q+p) \boldsymbol{a}_{1}+(2 q+p) \boldsymbol{a}_{2}
$$



Figure 1.2: a.) TBG at $\theta \sim 3.3^{\circ}$, which corresponds to $p=2$ and $q=19$. b.) TBG at $\theta \sim 21.8^{\circ}$, which corresponds to $p=1$ and $q=1$, and where red and blue lattices correspond to the underlying graphene sheets, and the dashed line illustrates the unit cell. c.) First BZ zone of TBG, where the red and blue hexagons represent the underlying graphene $B Z$ s with points $\boldsymbol{K}, \boldsymbol{K}^{\prime}, \boldsymbol{K}_{\theta}$ and $\boldsymbol{K}_{\theta}^{\prime}$, and the dashed hexagons are the $T B G B Z s$ with points $\boldsymbol{K}_{1}$ and $\boldsymbol{K}_{2}$.

Like graphene, the Brillouin zone of TBG is a hexagon with reciprocal lattice vectors

$$
\boldsymbol{G}_{1}=\frac{4}{N}\left((2 q+p) \boldsymbol{b}_{1}+(q+p) \boldsymbol{b}_{2}\right) \quad \text { and } \quad \boldsymbol{G}_{2}=\frac{4}{N}\left(-(q+p) \boldsymbol{b}_{1}+q \boldsymbol{b}_{2}\right)
$$

where $N=4\left(3 q^{2}+3 q p+p^{2}\right)$ is the number of sites in the TBG unit cell, and two in-equivalent corners

$$
\boldsymbol{K}_{1}=\left(\boldsymbol{G}_{1}+2 \boldsymbol{G}_{2}\right) / 3 \quad \text { and } \quad \boldsymbol{K}_{2}=\left(2 \boldsymbol{G}_{1}+\boldsymbol{G}_{2}\right) / 3
$$

Note that the last line holds for any $p$ and $q$. Since TBG inherits the two sets of graphene Dirac cones $\boldsymbol{K}, \boldsymbol{K}^{\prime}$ and $\boldsymbol{K}_{\theta}, \boldsymbol{K}_{\theta}^{\prime}$ of the first and second layer respectively, it is sensible to ask where they are located in the TBG Brillouin zone. For the case where $\operatorname{gcd}(p, 3)=1$, we have that $\boldsymbol{K}_{1}=\boldsymbol{K}=\boldsymbol{K}_{\theta}^{\prime}$ and $\boldsymbol{K}_{2}=\boldsymbol{K}^{\prime}=\boldsymbol{K}_{\theta}$, while for $\operatorname{gcd}(p, 3)=3$, we have $\boldsymbol{K}_{1}=\boldsymbol{K}=\boldsymbol{K}_{\theta}$ and $\boldsymbol{K}_{2}=\boldsymbol{K}^{\prime}=\boldsymbol{K}_{\theta}^{\prime}$. Hence, TBG has two doubly degenerate Dirac cones $\boldsymbol{K}_{1}$ and $\boldsymbol{K}_{2}$.

### 1.2.2 Band Structure

Although there are different analytical models for TBG, we will focus on the one presented by [2]. It describes the electronic properties close to the underlying graphene Dirac cones, and takes into account the hopping between the two layers. This model has the advantage to work for any shift $\boldsymbol{u}$ and any twist angle $\theta$, irrespective of whether such angle represents a commensurable structure.

This model considers the low energy dynamics of TBG around the two Dirac cones $\boldsymbol{K}_{1}$ and $\boldsymbol{K}_{2}$, and the Hamiltonian in real space can be written as

$$
H=\left(\begin{array}{cc}
-i v_{F} \boldsymbol{\sigma}^{-\theta / 2} \boldsymbol{\nabla} & \hat{T}(\boldsymbol{r})  \tag{1.7}\\
\hat{T}^{\dagger}(\boldsymbol{r}) & -i v_{F} \boldsymbol{\sigma}^{\theta / 2} \boldsymbol{\nabla}
\end{array}\right),
$$

where $\hat{T}$ is the real space hopping matrices, and $\boldsymbol{\sigma}^{\theta}$ are the rotated Pauli matrices (i.e $\boldsymbol{\sigma}^{\theta}=R(\theta) \boldsymbol{\sigma}$ where $R(\theta)$ is the rotation matrix and $\boldsymbol{\sigma}=\left(\sigma_{x}, \sigma_{y}\right)$ ). The matrix $\hat{T}(\boldsymbol{r})$ is the sum of many contributions which are calculated numerically. However, the authors of ref. [2] truncate the sum to include only the three most significant terms, in which case the matrix $\hat{T}(\boldsymbol{r})$ can be expressed as

$$
\hat{T}(\boldsymbol{r})=\sum_{j=1}^{3} e^{-i \boldsymbol{q}_{j} \boldsymbol{r}} T_{j}
$$

where we have

$$
\boldsymbol{q}_{1}=k_{\theta}(0,1), \quad \boldsymbol{q}_{2}=k_{\theta}(\sqrt{3} / 2,1 / 2) \quad \text { and } \quad \boldsymbol{q}_{3}=k_{\theta}(-\sqrt{3} / 2,1 / 2)
$$

with $k_{\theta}=\left(8 \pi / 3 a_{0}\right) \sin (\theta / 2)$, and the matrices

$$
T_{1}=\mathbb{1}+\sigma_{x}, \quad T_{2}=\mathbb{1}-\frac{1}{2} \sigma_{x}-\frac{\sqrt{3}}{2} \sigma_{y} \quad \text { and } \quad T_{3}=\mathbb{1}-\frac{1}{2} \sigma_{x}+\frac{\sqrt{3}}{2} \sigma_{y}
$$

where $\sigma_{x}$ and $\sigma_{y}$ are the Pauli matrices, and note that the matrices $T_{i}$ are hermitian.
In momentum space, where the momentum $\boldsymbol{k}$ is taken from the center of one Dirac cone, the Hamiltonian is

$$
H^{K}(\boldsymbol{k})=\left(\begin{array}{cccc}
h_{\theta / 2}^{K}(\boldsymbol{k}) & w T_{1} & w T_{2} & w T_{3}  \tag{1.8}\\
w T_{1}^{\dagger} & h_{-\theta / 2}^{K}\left(\boldsymbol{k}-\boldsymbol{q}_{1}\right) & 0 & 0 \\
w T_{2}^{\dagger} & 0 & h_{-\theta / 2}^{K}\left(\boldsymbol{k}-\boldsymbol{q}_{2}\right) & 0 \\
w T_{3}^{\dagger} & 0 & 0 & h_{-\theta / 2}^{K}\left(\boldsymbol{k}-\boldsymbol{q}_{2}\right)
\end{array}\right)
$$

where $h_{\theta}^{K}(\boldsymbol{k})$ is the graphene Dirac Hamiltonian around the $K$ point (eq. 1.3) rotated by the angle $\theta$, and $w \approx 0.11 \mathrm{eV}$ is the inter-layer hopping energy. This Hamiltonian is expected to give accurate results up to 1 eV and for $\theta<10^{\circ}$. The basis of this Hamiltonian is a four-vector of two-component spinors $\boldsymbol{\Psi}=\left(\psi_{0}, \psi_{1}, \psi_{2}, \psi_{3}\right)$, where $\psi_{0}$ is at the Dirac point of layer 1 , while the remaining $\psi_{j}$ are at momentum $\boldsymbol{q}_{j}$ and in layer 2. As shown in the original publication, the angle dependence of the graphene Dirac Hamiltonian can be neglected, and this is still expected to produce accurate results for $\theta$ larger than $\sim 1^{\circ}$.

The Hamiltonian of eq. 1.8 can be further simplified to a lower energy approximation by expanding around the Dirac cone of an isolated graphene layer. This is done by considering the momentum dependent and independent terms separately, and expanding the momentum dependent term to leading order in $\boldsymbol{k}$. It can be shown that $H_{0}^{K}$ has zero eigenvalues, such that only the momentum dependent term contributes. Hence, the low energy Hamiltonian around the center of the Dirac cone of one layer is

$$
\begin{equation*}
H_{\boldsymbol{k} \sim 0}^{K}(\boldsymbol{k})=\frac{-v_{F}}{1+6 \alpha^{2}}\left(\boldsymbol{\sigma} \cdot \boldsymbol{k}+w^{2} \sum_{j} T_{j} h^{-1 \dagger}\left(-\boldsymbol{q}_{j}\right) \boldsymbol{\sigma} \cdot \boldsymbol{k} h^{-1}\left(-\boldsymbol{q}_{j}\right) T_{j}^{\dagger}\right) \tag{1.9}
\end{equation*}
$$

where $h$ is used instead of $h^{K}, \alpha=w / v k_{\theta}$ and the sum is for values $j \in 1,2,3$. The first term in eq. 1.9 accounts for the isolated graphene Dirac cone, while the second term introduces the contribution from the neighbouring Dirac cones of the other layer. The term $1 /\left(1+6 \alpha^{2}\right)$ is for normalization purposes. Eq. 1.9 can be written as

$$
\begin{equation*}
H_{\boldsymbol{k} \sim 0}^{K}(\boldsymbol{k})=-v_{F}^{*} \boldsymbol{\sigma} \cdot \boldsymbol{k} \tag{1.10}
\end{equation*}
$$

where

$$
\begin{equation*}
v_{F}^{*}=\frac{1-3 \alpha^{2}}{1+6 \alpha^{2}} v_{F} \tag{1.11}
\end{equation*}
$$

is the renormalized Fermi velocity and $\alpha=w / v_{F} k_{\theta}$. The eigenvalues are

$$
\begin{equation*}
\epsilon_{\boldsymbol{k} \sim 0}= \pm v_{F}^{*}|\boldsymbol{k}| . \tag{1.12}
\end{equation*}
$$

Eq. 1.8 is not guaranteed to have analytical solutions, since it is an $8 \times 8$ matrix, and there is not guaranteed solution for polynomial equations of order higer than 5. For this reason, eq. 1.8 is


Figure 1.3: Numerical solution to eq. 1.8 (solid line), and analytical solution to eq. 1.10 (dotted line), for $\theta \in\left\{1.05^{\circ}, 5^{\circ}\right\}$ along the $k_{x}$ and $k_{y}$ axis, and $a$ is the carbon-carbon distance in graphene.
diagonalized numerically, and the results are shown with the solid line in fig. 1.3, for $\theta=5^{\circ}$ and $\theta=1.05^{\circ}$, and the spectrum is along both $k_{x}$ and $k_{y}$. The dotted line shows the approximation resulting from the Hamiltonian of eq. 1.10. For $\theta=5^{\circ}$, the emergent Dirac cone is clearly present, and the approximation holds well for energies up to $\epsilon \sim 0.2 \mathrm{eV}$. For $\theta=1.05^{\circ}$ however, the Dirac cone is absent, and the lowest bands are in fact flat, as expected in a superconducting system. In this case, the low energy approximation is not as good, and is in principle not justified since the Dirac cone is not present.

## Chapter 2

## Quantum Oscillations

In this chapter, we introduce quantum oscillations, by first presenting the relevant classical theory, on which we then enforce quantization to then demonstrate the emergence of the oscillations. Finally, we consider the application to graphene and twisted bilayer graphene (TBG). The theory presented is largely based on refs. $[13,32]$.

### 2.1 Electrons in a Magnetic Field

The dynamics of a charged particle, in this case an electron, can be obtained through the Lorentz force

$$
\begin{equation*}
\dot{\boldsymbol{k}}=e(\boldsymbol{v} \times \boldsymbol{H}), \tag{2.1}
\end{equation*}
$$

where $\boldsymbol{k}$ is the electron wave vector, $\boldsymbol{v}$ is the electron velocity, $\boldsymbol{H}$ is the magnetic field, $c$ is the speed of light and $-e$ is the electron charge. The relationship between the electron velocity and the energy $\epsilon$ is

$$
\begin{equation*}
\boldsymbol{v}=\nabla_{k} \epsilon . \tag{2.2}
\end{equation*}
$$

From the above equation, we can see that $\boldsymbol{v}$ is normal to a surface of constant energy ${ }^{1}$, and therefore $\dot{\boldsymbol{k}}$ is tangent to a surface of constant energy. Since $\dot{\boldsymbol{k}}$ is also normal to $\boldsymbol{H}$, it follows that $\boldsymbol{k}$ will move along a surface of constant energy on a plane perpendicular to $\boldsymbol{H}$.

By integrating both sides, we get

$$
\begin{equation*}
\left(\boldsymbol{k}-\boldsymbol{k}_{0}\right)=-e\left(\boldsymbol{R}-\boldsymbol{R}_{0}\right) \times \boldsymbol{H} \tag{2.3}
\end{equation*}
$$

where $\boldsymbol{R}$ is the electron position in real space, and $\boldsymbol{k}_{0}$ and $\boldsymbol{R}_{0}$ are constants of integration. This shows that the electron position projected on a plane perpendicular to $\boldsymbol{H}$ describes a scaled version of the motion of the wave vector. Note however that the electron can still travel in the direction of the magnetic field. In other words, the motion of the electron in real space can be helical. However, if we let $\boldsymbol{R}_{\perp}$ be the projection of $\boldsymbol{R}$ on a plane perpendicular to $H$, we get

$$
\begin{equation*}
\left|\boldsymbol{k}-\boldsymbol{k}_{0}\right|=e H\left|\boldsymbol{R}-\boldsymbol{R}_{0}\right|, \tag{2.4}
\end{equation*}
$$

giving the relative scaling between the real-space and momentum space orbits.

[^0]Before we move on, we shall also define the cyclotron frequency,

$$
\begin{equation*}
\omega_{c}=2 \pi e H /\left(\frac{\partial a}{\partial \epsilon}\right)_{\boldsymbol{k}_{\|}} \tag{2.5}
\end{equation*}
$$

where $a$ is the area in momentum space that the $\boldsymbol{k}$ orbit describes, and $\boldsymbol{k}_{\|}$signifies that the component of $\boldsymbol{k}$ along $H$ is kept constant in the derivative. A derivation of eq. 2.5 is beyond the scope of this thesis.

### 2.2 Quantization of Orbits in a Magnetic Field

We must now treat the above theory in the framework of quantum mechanics, in which the electron orbits must be quantized. We assume that the orbits of particles in a magnetic field are quantized according to the Bohr-Sommerfeld semiclassical relation

$$
\begin{equation*}
\oint \boldsymbol{p} \cdot d \boldsymbol{r}=2 \pi(n+\gamma) \tag{2.6}
\end{equation*}
$$

where the integral is taken over a complete orbit, $n$ is an integer, and $\gamma$ is the phase correction, which is $\gamma=1 / 2$ for parabolic bands and $\gamma=0$ for graphene. Furthermore, $\boldsymbol{p}$ and $\boldsymbol{r}$ are the canonical momentum and position respectively. For an electron in a magnetic field, we have $\boldsymbol{r}=\boldsymbol{R}_{\perp}$ as the position perpendicular to $\boldsymbol{H}$ and the momentum $\boldsymbol{p}$ as the sum of the kinetic $\boldsymbol{p}_{\text {kin }}=m \boldsymbol{v}=\boldsymbol{k}$ and the field momentum $\boldsymbol{p}_{\text {field }}=-e \boldsymbol{A}$, where $e$ is the charge of an electron and we have that $\boldsymbol{H}=\nabla \times \boldsymbol{A}$. Hence, the total momentum is

$$
\begin{equation*}
\boldsymbol{p}=\boldsymbol{p}_{\text {kin }}+\boldsymbol{p}_{\text {field }}=\boldsymbol{k}-e \boldsymbol{A} \tag{2.7}
\end{equation*}
$$

and substituting in eq. 2.6 we have

$$
\oint \boldsymbol{k} \cdot d \boldsymbol{R}_{\perp}-e \oint \boldsymbol{A} \cdot d \boldsymbol{R}_{\perp}=2 \pi(n+\gamma) .
$$

Using eq. 2.3 to transform the first term (the constants of integration account for nothing), and Stokes' theorem for the second, we get

$$
\boldsymbol{H} \cdot \oint \boldsymbol{R} \times d \boldsymbol{R}_{\perp}-\int_{S} \boldsymbol{H} \cdot d \boldsymbol{S}=2 \pi(n+\gamma) / e
$$

where $S$ denotes an area in real space. For the first term, we have also used that the scalar triple product remains unchanged under a circular shift and that the cross product is anti-commutative. Finally, we get

$$
\Phi=2 \pi(n+\gamma) / e
$$

where $\Phi=\boldsymbol{H} \cdot \boldsymbol{S}$ is the magnetic flux and for the first term, we used the geometrical result

$$
\oint \boldsymbol{r} \times d \boldsymbol{r}=2 \times(\text { area enclosed by orbit }) .
$$

Hence, the Bohr-Sommerfeld rule ensures that the magnetic flux $\Phi$ through the real-space orbit described by an electron is quantized. To get the quantization rule in momentum space, we use eq. 2.4 to get the momentum-space area $a=(e H)^{2} S$, and hence we have

$$
\begin{equation*}
a(\epsilon)=2 \pi e H(n+\gamma) \tag{2.8}
\end{equation*}
$$

where the dependence of $a$ on $\epsilon$ is stressed. Eq. 2.8 is most known as the Onsager relation, and specifies what energies an electron is allowed to have in a magnetic field. In other words, for a given $H, n$ and $\gamma$, the Onsager relation dictates the specific surface area $a$ the orbit of an electron must obey.


Figure 2.1: a). Number of particles $N$ that are in orbits which are fully occupied (gray region), where $N-100$ is the number of particles in partially filled orbits (white region) for a system with 100 particles, and $H$ is the magnetic field. b.) Identical to a.) except plotted with respect to the inverse magnetic field $1 / H$.

### 2.3 De Haas-Van Alphen Effect

The de Haas-van Alphen effect reffers to oscillations observed in the magnetic moment of a metal. In this section, we will establish the physical reason why such oscillations occur for systems in 2 dimensions. For 2 dimensions, we are essentially dealing with a restriction on the more general 3 dimensional case. Certain extra technical details occur in 3 dimensional systems, but we will not consider them in this thesis.

In a 2 dimensional solid, and neglecting spin, the area in momentum space occupied by an electron in the case $\boldsymbol{H}=0$ is $(2 \pi / L)^{2}$, where $L$ is the real space length of the sample assumed to be square. The number of states (neglecting spin) allowed per orbit is equal to the area between orbits times the number of states per unit area for $\boldsymbol{H}=0$. From eq. 2.9, the area between two successive orbits for a set value of $\boldsymbol{H}$ is

$$
\begin{equation*}
a_{n+1}(\epsilon)-a_{n}(\epsilon)=2 \pi e H \tag{2.9}
\end{equation*}
$$

Hence, the degeneracy $D$ for a single orbit is

$$
\begin{equation*}
D=2 \pi e H(L / 2 \pi)^{2}=\rho H \tag{2.10}
\end{equation*}
$$

where $\rho=e L / 2 \pi$. Then, for a system with $N$ particles, the first $D n$ particles will reside in fully filled orbits, where $n$ refers to the number of filled orbits, while the remaining $N-D n^{\prime}$ particles will occupy the last $n+1$ orbit. At specific values of $H$, all particles will reside in filled orbits, such that $D n=N$. We find that the interval between $H_{n}$ and $H_{n+1}$, magnetic fields where exactly all $n$ and $n+1$ orbits are filled, is

$$
\begin{equation*}
\frac{1}{H_{n+1}}-\frac{1}{H_{n}}=\frac{\rho}{N} . \tag{2.11}
\end{equation*}
$$

The imporant feature of eq. 2.11 is that it is constant with respect to $1 / H$, as can be seen in fig. 2.1. Thus, there is a singularity in the energy that occurs periodically with $1 / H$, and this is the nature of de Haas-van Alphen oscillations, and of quantum oscillations in general.

### 2.4 Example with Graphene

In order to illustrate the theory established above, we shall consider the case for graphene, more precisely the low energy Dirac equation. From section 1.1, eq. 1.4, we have

$$
\epsilon_{ \pm}(\boldsymbol{k})= \pm v_{F}|\boldsymbol{k}|
$$

where the surface of constant $\epsilon$ are discs with radius $|\boldsymbol{k}|$. Hence, the area of the discs are $a=\pi k^{2}$, and the energy can then be written as

$$
\epsilon= \pm v_{F} \sqrt{a / \pi}
$$

It follows directly from eq. 2.8 that in a magnetic field, the allowed eigenstates are

$$
\begin{equation*}
\epsilon= \pm v_{F} \sqrt{2 e H n}= \pm \omega_{B} \sqrt{n}, \tag{2.12}
\end{equation*}
$$

where $\gamma=0$, and it is common to define $\omega_{B}=\sqrt{2} v_{F} / l_{B}$ and the magnetic length $l_{B}=1 / \sqrt{e H}$. However, using eq. 2.5, we have for graphene

$$
\omega_{c}=e H v_{F}^{2} / \epsilon
$$

which is inversely proportional to energy, unlike $\omega_{c}$ for parabolic bands for example. This is because the spacing between the orbits is not constant for graphene, due to the square root dispersion. However, we can interpret $\omega_{B}$ as the spacing between the first and the second orbit (i.e. between $n=0$ and $n=1$ ), such that $\omega_{B}$ is the quantum limit of $\omega_{c}$. Nevertheless, throughout this thesis, we will use $\omega_{c}$ to refer to $\omega_{B}$, such that $\omega_{c}=v_{F} \sqrt{2 e H}$, since it is commonly done in other texts.

### 2.5 Twisted Bilayer Graphene

As previously pointed out, eq. 1.8 is not guaranteed an analytical solution, and we can therefore not apply the theory derived in section 2.2 . The consequence of this is that we must find a numerical method to compute the spectrum of TBG in a magnetic field, and this will be discussed in the next chapter. Nevertheless, we can obtain an analytical solution to the low energy approximation of eq. 1.10, which gives

$$
\begin{equation*}
\epsilon= \pm v_{F}^{*} \sqrt{2 e H n}, \tag{2.13}
\end{equation*}
$$

where $v_{F}^{*}$ is the renormalized Fermi velocity from eq. 1.11.

## Chapter 3

## Numerical Method

As mentioned in the previous chapter, the twisted bilayer graphene (TBG) Hamiltonian is too difficult to diagonalize analytically, and we must proceed numericaly. In this section, we present a numerical scheme based on [4], through which we could in principle obtain the Landau levels of any system, given that we know its Hamiltonian expressed in terms of ladder operators. Using this numerical scheme, we also explain why it is difficult to obtain an analytical solution for TBG in a magnetic field. Finally, we present the numerical results and discuss a possible analytical approximation.

### 3.1 Quantization Using Ladder Operators

As previously mentioned, the momentum of an electron in a magnetic field is $(\hbar=c=1)$

$$
\boldsymbol{p}=\boldsymbol{p}_{\text {kin }}+\boldsymbol{p}_{\text {field }}=\boldsymbol{k}-e \boldsymbol{A}
$$

where $-e$ is the charge of the electron and $\boldsymbol{A}=-y B \hat{\boldsymbol{e}}_{x}$ is the Landau gauge. Because in quantum mechanics $k_{x}$ and $x$ do not commute, we expect $\left[p_{x}, p_{y}\right] \neq 0$. Indeed, we get

$$
\left[p_{x}, p_{y}\right]=\left[k_{x}+e B y, k_{y}\right]=i e B
$$

where we used that $\left[y, k_{y}\right]=i$. Hence, $\left[p_{x}, p_{y}\right]$ is equal to $\left[x, k_{x}\right]$ neglecting a factor of $e B$. This suggests that the physics is essentially the same as the quantum harmonic oscillator, and can be solved using ladder operators. Thus, we define the creation and annihilation operators as

$$
\hat{a} \propto p_{x}-i p_{y} \quad \text { and } \quad \hat{a}^{\dagger} \propto p_{x}+i p_{y}
$$

as in the quantum harmonic oscillator, and where the constant of proportionality is found by enforcing $\left[\hat{a}, \hat{a}^{\dagger}\right]=1$. Indeed, we get

$$
\left[\hat{a}, \hat{a}^{\dagger}\right]=2 i\left[p_{x}, p_{y}\right]=2 e B
$$

which means that we have

$$
\hat{a}=\frac{1}{\sqrt{2 e B}}\left(p_{x}-i p_{y}\right) \quad \text { and } \quad \hat{a}^{\dagger}=\frac{1}{\sqrt{2 e B}}\left(p_{x}+i p_{y}\right)
$$

In the case of an electron in a magnetic field, the ladder operators act on a Landau level, where $\hat{a}$ $\left(\hat{a}^{\dagger}\right)$ decreases (increases) the Landau level of the particle by one. Their eigenvalues are

$$
\hat{a}|n\rangle=\sqrt{n}|n-1\rangle \quad \text { and } \quad \hat{a}^{\dagger}|n\rangle=\sqrt{n+1}|n+1\rangle .
$$

We can now express the momentum operators in terms of ladder operators. We obtain

$$
\begin{equation*}
p_{x}=\frac{1}{2} \sqrt{2 e B}\left(\hat{a}+\hat{a}^{\dagger}\right) \quad \text { and } \quad p_{y}=\frac{i}{2} \sqrt{2 e B}\left(\hat{a}-\hat{a}^{\dagger}\right) . \tag{3.1}
\end{equation*}
$$

The Hamiltonian of a particle in a magnetic field can now be expressed in terms of $\hat{a}$ and $\hat{a}^{\dagger}$ by substituting the above equations. In some cases, the Hamiltonian can then be solved analytically, such as the case for a 2D electron gas or graphene. In other cases, it is still too difficult to solve analytically, and further work has to be done. In our case, we assume that our system is too complicated to solve analytically, and we consider a numerical technique to solve a Hamiltonian expressed in terms of ladder operators.

### 3.2 Numerical Implementation of Ladder Operators

To numerically solve any arbitrary Hamiltonian expressed in terms of ladder operators, we must express the ladder operators $\hat{a}$ and $\hat{a}^{\dagger}$ as square matrices $\boldsymbol{A}$, and $\boldsymbol{A}^{\dagger}$ of dimension $N \times N$. The matrices act on a basis of $N$ Landau levels, where $N$ is an arbitrary cutoff, and the matrix elements

$$
\begin{gathered}
A_{n, m}:=\langle n| \hat{a}|m\rangle=\delta_{n, m+1} \sqrt{m} \text { and } \\
A_{n, m}:=\langle n| \hat{a}^{\dagger}|m\rangle=\delta_{n, m-1} \sqrt{n}
\end{gathered}
$$

are obtained by the above equations. For $N=3$, we have

$$
\boldsymbol{A}=\left(\begin{array}{ccc}
0 & 1 & 0 \\
0 & 0 & \sqrt{2} \\
0 & 0 & 0
\end{array}\right), \quad \text { and } \quad \boldsymbol{A}^{\dagger}=\left(\begin{array}{ccc}
0 & 0 & 0 \\
1 & 0 & 0 \\
0 & \sqrt{2} & 0
\end{array}\right)
$$

The numerical scheme, requires the Hamiltonian to be decomposed as a polynomial in powers of $\hat{a}$ and $\hat{a}^{\dagger}$. The Kronecker product is then taken between the matrix ladder operators $\boldsymbol{A}$, and $\boldsymbol{A}^{\dagger}$ and their respective coefficients, and finally added together. For the term which is the zeroth power in ladder operators, the Kronecker product is taken with the unit matrix of dimension $N \times N$. To illustrate, consider the example Hamiltonian

The numerical scheme requires to first express the Hamiltonian in terms of $\hat{a}$ and $\hat{a}^{\dagger}$ operators, and then to separate the equation in powers of the operators. The final matrix is obtained by taking the Kronecker product between the ladder operators in matrix form and their coefficients, and adding them together. Consider the example

$$
H=\left(\begin{array}{cc}
c & \hat{a}^{\dagger} \\
\hat{a} & c
\end{array}\right)=(\hat{a})\left(\begin{array}{ll}
0 & 0 \\
1 & 0
\end{array}\right)+\left(\hat{a}^{\dagger}\right)\left(\begin{array}{ll}
0 & 1 \\
0 & 0
\end{array}\right)+\left(\begin{array}{ll}
c & 0 \\
0 & c
\end{array}\right)
$$

which has been deconstructed into a polynomial of ladder operators, and where $c$ is an arbitrary constant. The resulting 'augmented' Hamiltonian $H$ will therefore be

$$
\boldsymbol{H}=\boldsymbol{A} \otimes\left(\begin{array}{ll}
0 & 0 \\
1 & 0
\end{array}\right)+\boldsymbol{A}^{\dagger} \otimes\left(\begin{array}{ll}
0 & 1 \\
0 & 0
\end{array}\right)+\mathbb{1} \otimes\left(\begin{array}{ll}
c & 0 \\
0 & c
\end{array}\right)
$$

where $\mathbb{1}$ is the unit matrix of dimension $N \times N$. Due to the Kronecker product, the Hamiltonian $H$ will have a dimension greater than $N(2 N \times 2 N$ in this case $)$, and is generally equal to $N \times$ (dim. of $H$ ). It then suffices to diagonalize $\boldsymbol{H}$ numerically using any suitable implementation.


Figure 3.1: a.) Numerical solution for $H_{K}$ with $N \in\{10,20,30\}$ Landau levels, the solid line is the analytical solution, and we have used $\omega_{c}=1.0$. b.) same as a.) but with $H_{K, \text { shift }}$.

### 3.2.1 Example with Graphene

From section 2.4, we already established that low energy eigenvalues of graphene (eq. 1.4) lead to eigenvalues $\sim \sqrt{n}$ (eq. 2.12) in a magnetic field $H$, where the integer $n$ is the Landau level index. We can also arrive to this result using the previously defined Ladder operators, and using eq. 1.3 for the $K$ Dirac cone along with the momentum substitutions from eq. 3.1, we get

$$
H_{K}=v_{F} \sqrt{2 e H}\left(\begin{array}{cc}
0 & \hat{a}  \tag{3.2}\\
\hat{a}^{\dagger} & 0
\end{array}\right) .
$$

To solve this equation, we assume $(|n\rangle, \pm|m\rangle)$ as the form of the eigenvectors, which leads to eigenvectors $(|n-1\rangle, \pm|n\rangle)$ with eigenvalues

$$
\begin{equation*}
\epsilon= \pm v_{F} \sqrt{2 e H n} \tag{3.3}
\end{equation*}
$$

identical to eq. 2.12. For the $K^{\prime}$ Dirac cone, this amounts to the switch $\hat{a} \leftrightarrow \hat{a}^{\dagger}$ in eq. 3.2, which leads to eigenvectors $(|n\rangle, \pm|n-1\rangle)$ but identical eigenvalues. To diagonalize eq. 3.3 numerically, one follows the scheme laid out in section 3.2 , which gives a $2 N \times 2 N$ matrix, where $N$ is the highest Landau level considered. The resulting positive ${ }^{1}$ eigenvalues are presented in fig. 3.1(a) for $N=10,20$ and 30 , along with the analytical solution given in eq. 3.3.

For further interest, we can apply an arbitrary momentum shift $\boldsymbol{q}$ to eq. 3.2, such that

$$
H_{K, \text { shift }}=v_{F} \sqrt{2 e H}\left(\begin{array}{cc}
0 & \hat{a}+\boldsymbol{q}  \tag{3.4}\\
\hat{a}^{\dagger}+\boldsymbol{q}^{*} & 0
\end{array}\right)
$$

where $\boldsymbol{q}^{*}$ is the complex conjugate of $\boldsymbol{q}$. The numerical result is illustrated in fig. 3.1(b) for same values of $N$. Eq. 3.4 can also be diagonalized analytically, and yields the same result as eq. 3.2 , since the added momentum terms can be absorbed into $\boldsymbol{k}$ by an adequate shift. However, the numerical result only seems to be correct for Landau levels that are much smaller than the cutoff $N$. Hence, the numerical result for a given Landau level $n$ is not guaranteed exact but converges as $N \rightarrow \infty$.

### 3.2.2 Difficulty in Obtaining Landau Levels Analytically for TBG

As previously mentioned in section 2.5 , it is difficult to obtain the eigenvalues of eq. 1.8 analytically. Using ladder operators and the numerical scheme laid out above, we can further understand the origin of this difficulty. First, we consider the previous Hamiltonian for graphene in a magnetic field

[^1]from eq. 3.2, where we neglect leading factors. We can apply the numerical procedure to get the following eigenvalue equation
\[

\left($$
\begin{array}{cccccc}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \sqrt{2} & 0 \\
0 & 0 & 0 & \sqrt{2} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{array}
$$\right)\left($$
\begin{array}{c}
|0, a\rangle \\
|0, b\rangle \\
|1, a\rangle \\
|1, b\rangle \\
|2, a\rangle \\
|2, b\rangle
\end{array}
$$\right)=\epsilon\left($$
\begin{array}{l}
|0, a\rangle \\
|0, b\rangle \\
|1, a\rangle \\
|1, b\rangle \\
|2, a\rangle \\
|2, b\rangle
\end{array}
$$\right)
\]

where $|0, a\rangle$ referes to the $0^{\text {th }}$ Landau level on sublattice $a$, and we have arbitrarily truncated the matrix to keep only the first 3 Landau levels. Solving for $\epsilon$ amounts to solving the 6 equations

$$
\begin{array}{lll}
0=\epsilon|0, a\rangle, & |1, a\rangle=\epsilon|0, b\rangle, & \sqrt{2}|2, a\rangle=\epsilon|1, b\rangle, \\
0=\epsilon|2, b\rangle, & |0, b\rangle=\epsilon|1, a\rangle, & \sqrt{2}|1, b\rangle=\epsilon|2, a\rangle,
\end{array}
$$

where the equations in the first column depend on $|0, a\rangle$ and $|2, b\rangle$, the second column on $|1, a\rangle$ and $|0, b\rangle$, and the third on $|2, a\rangle$ and $|1, b\rangle$. Hence, the equations are grouped such that they only depend on a few variables that are only present in those equations. This feature is a consequence of the fact that the above matrix can be decomposed into block matrices along its diagonal. This makes the equations easily solvable, where the first column leads to $\epsilon=0$, the second to $\epsilon=1$ and so forth. If we now consider the Hamiltonian for graphene with a shift from eq. 3.4, and apply the same procedure, we get the following equation

$$
\left(\begin{array}{cccccc}
0 & q & 0 & 0 & 0 & 0 \\
q & 0 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & q & 0 & 0 \\
0 & 0 & q & 0 & \sqrt{2} & 0 \\
0 & 0 & 0 & \sqrt{2} & 0 & q \\
0 & 0 & 0 & 0 & q & 0
\end{array}\right)\left(\begin{array}{l}
|0, a\rangle \\
|0, b\rangle \\
|1, a\rangle \\
|1, b\rangle \\
|2, a\rangle \\
|2, b\rangle
\end{array}\right)=\epsilon\left(\begin{array}{l}
|0, a\rangle \\
|0, b\rangle \\
|1, a\rangle \\
|1, b\rangle \\
|2, a\rangle \\
|2, b\rangle
\end{array}\right)
$$

where we considered that $q$ is real such that $q^{*}=q$. In this case, it is impossible to decompose the above matrix into block matrices due to the introduction of $q$. The consequence is that any of the resulting 6 equations will depend on the other 5 , such that solving for one equation requires solving all. This technical problem can be resolved by applying a shift to the momentum $\boldsymbol{k}$ prior to introducing the ladder operators, but it does explain the convergence requirement explained in the previous subsection.

If we now consider the TBG Hamiltonian from eq. 1.8, we see that it does contain Dirac Hamiltonians with a shift. However, it is not possible to eliminate this shift since the Dirac Hamiltonians are connected to each other by off diagonal terms. In principle, if the off diagonal elements are small enough to be neglected, the TBG Hamiltonian is solvable. This is the case for high magnetic fields for example, but this would require $\omega_{c} \sim 100$.

### 3.2.3 Numerical Computation of TBG Landau Levels

We now apply the above numerical scheme to to our TBG model, using eq. 1.8. The result is shown in fig. 3.2 for the first 50 Landau levels, with $\omega_{c} \in\{10,1,0.1,0.03\}$ and $\theta \in\left\{5^{\circ}, 1.05^{\circ}\right\}$. The dashed line represents the high energy approximation and corresponds to $\sqrt{n / 4}$, and the insets show the difference between the approximation and the numerical results. The approximation is


Figure 3.2: Numerical solution to the TBG Hamiltonian in a magnetic field using the aforementioned method for $\omega_{c} \in\{10.0,1.0,0.1,0.03\}$, and for $\theta \in\left\{1.05^{\circ}, 5^{\circ}\right\}$, and where the dashed line represents the approximation mentionned in the text. The results are shown for the first 50 Landau levels, and the matrices were truncated at 2000 Landau levels. The insets show the difference between the analytical approximation and the numerical solution for the first 500 Landau levels in all cases except for $\omega_{c}=0.03$, for which the inset includes the first 1000 Landau levels.


Figure 3.3: a.) and b.) Numerical results of TBG in a magnetic field compared to the low energy approximation from eq.1.10 at $\omega_{c}=0.03$ for $\theta=1.05^{\circ}$ and $\theta=5^{\circ}$ respectively. c.) Percentage error between the $400^{\text {th }}$ Landau level obtained using a cutoff $N$ and the $400^{\text {th }}$ Landau level obtained using $N=2000$. Results are presented only for the lowest values of $\omega_{c}$, since the convergence is almost guaranteed for high $\omega_{c}$.
justified since it corresponds to the spectrum in the case where the Dirac cones are uncoupled. In such case, the Landau levels would behave as $\sqrt{n}$, where we include a factor of $\sqrt{1 / 4}$ to account for the degeneracy.It is important to note however that eq. 1.8 is only valid for $\epsilon<1 \mathrm{eV}$, such that only the case when $\omega_{c} \in\{0.1,0.03\}$ is valid.

First of all, we note that for $\omega_{c}=10$, the spectrum does behave as if the Dirac cones were uncoupled, as mentioned previously. In this case, the spectrum is analogous to that of graphene, except with an extra degeneracy factor of 4 clearly seen in fig. 3.2 (a) and (b). The results seem to agree with the approximation for $\omega_{c} \in\{10,1\}$ for low Landau levels already ( $n \sim 50$ ). For $\omega_{c}=0.1$, the approximation differs somewhat, but only for low Landau levels, as shown by the insets of fig. 3.2 (e) and (f). For $\omega_{c}=0.03$, the approximation holds well for $\theta=5^{\circ}$ at relatively low Landau level, but as seen in the inset of fig. 3.2 (g), the numerical results do not show an obvious convergence towards the approximation even for the $1000^{\text {th }}$ Landau level. For $\theta=1.05^{\circ}$, the low Landau level range differs somewhat from the approximation, but eventually converges towards the approximation.

Fig. 3.3 (a) and (b) show the first 50 Landau levels for $\theta=1.05^{\circ}$ and $\theta=5^{\circ}$ respectively, compared to the low energy approximation from eq. 1.10, illustrated as the dashed line. The low energy approximation holds well for $\theta=5^{\circ}$, as expected since the Dirac cone picture of TBG good for this angle up to energies of $\epsilon \sim 0.2 \mathrm{eV}$. However, for $\theta=1.05^{\circ}$, the low energy approximation is accurate only for the first few Landau levels, as expected since there is technically no Dirac cone at the magic angle. Fig. 3.3(c) illustrates the percentage in error of the $400^{\text {th }}$ Landau level for $\omega_{c} \in\{0.1,0.03\}$, and demonstrates the limit of the numerical method. Obtaining results for $/$ theta $=5^{\circ}$ proves very difficult above $\omega_{c}=0.03$ since the convergence would require 2000 Landau levels, and considering any more Landau levels greatly increases the computational time from minutes to hours, causing the computational time for quantum oscillations to go from hours to months as we will see in the results chapter.

## Chapter 4

## Lifshitz-Kosevich Formula

From the previous section, we obtained an analytical solution for twisted bilayer graphene (TBG) in a magnetic field. I this section, we therefore introduce the Lifshitz-Kosevich formula, which is an analytical way of obtaining the frequency and amplitude quantum oscillations. We then derive the results for graphene and TBG following ref. [28].

### 4.1 General Case

The grand potential of a system can be expressed in terms of the system's Green's function by the Luttinger-Ward functional $\left(\hbar=c=k_{B}=1\right)$

$$
\Omega=-T \operatorname{tr}\left[\ln \left(-\hat{G}^{-1}\right)\right]-T \operatorname{tr}[\hat{G} \hat{\Sigma}]+\Omega^{\prime}
$$

where $T$ is the temperature, the trace implies the sum over all energy states as well as the fermionic Matsubara frequencies $\omega_{n}=\pi T(2 n+1)$, and the self-energy $\Sigma$ accounts for disorder and interaction effects. In the absence of disorder or interactions, the terms $T \operatorname{tr}[\hat{G} \hat{\Sigma}]$ and $\Omega^{\prime}$ do not contribute, and we have

$$
\begin{equation*}
\Omega=-T \operatorname{tr}\left[\ln \left(-\hat{G}^{-1}\right)\right]=-D T \sum_{m=0}^{\infty} \sum_{\omega_{n}} \ln \left(-g_{m}^{-1}\left(i \omega_{n}\right)\right), \tag{4.1}
\end{equation*}
$$

where we used that the trace of a diagonalizable matrix is equal to the sum of its eigenvalues, and where $g_{m}\left(i \omega_{n}\right)$ are the eigenvalues of $\hat{\hat{G}}$. The index $m$ represents the $m^{\text {th }}$ Landau level, and the sum over the Matsubara frequencies runs from $n=-\infty$ to $n=\infty$. Lastly, we introduced a degeneracy factor $D$ to account for the fact that the sum over $m$ counts each Landau level only once.

To compute the sum over $m$, we can use the Poisson summation formula derived in Appendix A,

$$
\sum_{n=0}^{\infty} f(n)=\int_{0}^{\infty} \mathrm{d} x f(x) \sum_{l=-\infty}^{\infty} e^{i 2 \pi l x}=\int_{0}^{\infty} \mathrm{d} x f(x)+2 \sum_{l=1}^{\infty} \int_{0}^{\infty} \mathrm{d} x f(x) \cos (2 \pi l x)
$$

where we used that $2 \cos (x)=e^{i x}+e^{-i x}$ for the last equality. The first term of the last equality is neglected since it does not contribute to the oscillations, and hence we have

$$
\Omega_{\mathrm{osc}}=-2 D T \sum_{l=1}^{\infty} \sum_{\omega_{n}} \int_{0}^{\infty} \mathrm{d} x \ln \left(-g^{-1}\left(x, i \omega_{n}\right)\right) \cos (2 \pi l x)
$$

where $x$ indicates a continuous analog to the Landau level index $m$, and where $\Omega_{\text {osc }}$ only referes to the oscillatory part of $\Omega$.

Integrating by parts gives us

$$
\begin{aligned}
\Omega_{\mathrm{osc}}= & -2 D T \sum_{l=1}^{\infty} \sum_{\omega_{n}}\left[\ln \left(-g^{-1}\left(x, i \omega_{n}\right)\right) \frac{\sin (2 \pi l x)}{2 \pi l}\right]_{0}^{\infty} \\
& +2 D T \sum_{l=1}^{\infty} \sum_{\omega_{n}} \int_{0}^{\infty} \mathrm{d} x \frac{1}{-g^{-1}\left(x, i \omega_{n}\right)} \frac{\mathrm{d}}{\mathrm{~d} x}\left(-g^{-1}\left(x, i \omega_{n}\right)\right) \frac{\sin (2 \pi l x)}{2 \pi l}
\end{aligned}
$$

and since the first term is non-oscillatory, we are left with

$$
\Omega_{\mathrm{osc}}=2 D T \sum_{l=1}^{\infty} \sum_{\omega_{n}} \int_{0}^{\infty} \mathrm{d} x \frac{1}{-g^{-1}\left(x, i \omega_{n}\right)} \frac{\mathrm{d}}{\mathrm{~d} x}\left(-g^{-1}\left(x, i \omega_{n}\right)\right) \frac{\sin (2 \pi l x)}{2 \pi l}
$$

### 4.2 Graphene

We will now derive the Lifshitz-Kosevich (LK) formula for graphene, neglecting any disorder or interaction effects. The inverse non-interacting Green's function $\hat{G}_{0}^{-1}$ is

$$
\hat{G}_{0}^{-1}=\left(i \omega_{n}+\mu\right) \mathbb{1}-\hat{H}
$$

where $\omega_{n}=\pi T(2 n+1)$ are the Matsubara frequencies, and the Hamiltonian for graphene is

$$
\hat{H}=\left(\begin{array}{cc}
0 & \omega_{c} \sqrt{m} \\
\omega_{c} \sqrt{m} & 0
\end{array}\right)
$$

where $m$ is the Landau level index. Hence, we have

$$
\hat{G}_{0}^{-1}=\left(\begin{array}{cc}
i \omega_{c}+\mu & \omega_{c} \sqrt{m} \\
\omega_{c} \sqrt{m} & i \omega_{c}+\mu
\end{array}\right)
$$

and the eigenvalues of this matrix are

$$
g_{m, \pm}^{-1}=i \omega_{n}+\mu \pm \omega_{c} \sqrt{m}
$$

The grand potential is then

$$
\begin{aligned}
\Omega_{\mathrm{osc}} & =2 D T \sum_{l=1}^{\infty} \sum_{\omega_{n}} \sum_{\lambda= \pm 1} \int_{0}^{\infty} \mathrm{d} x \frac{1}{i \omega_{n}+\mu+\lambda \omega_{c} \sqrt{x}} \frac{\lambda \omega_{c}}{2 \sqrt{x}} \frac{\sin (2 \pi l x)}{2 \pi l} \\
& =2 D T \sum_{l=1}^{\infty} \sum_{\omega_{n}} \int_{0}^{\infty} \mathrm{d} x \frac{\sin (2 \pi l x)}{2 \pi l} \frac{\omega_{c}}{2 \sqrt{x}}\left\{\frac{1}{i \omega_{n}+\mu+\omega_{c} \sqrt{x}}+\frac{1}{-i \omega_{n}-\mu+\omega_{c} \sqrt{x}}\right\} \\
& =2 D T \sum_{l=1}^{\infty} \sum_{\omega_{n}} \int_{0}^{\infty} \mathrm{d} x \frac{\sin (2 \pi l x)}{2 \pi l} \frac{\omega_{c}}{2 \sqrt{x}} \frac{2 \omega_{c} \sqrt{x}}{\omega_{c}^{2} x-\left(i \omega_{n}+\mu\right)^{2}}
\end{aligned}
$$

where we used a sum over $\lambda$ to account for the ' $\pm$ ' sign, and expanded the sum in the second equality. For the third equality, we used $1 /(A+B)+1 /(A-B)=2 A /\left(A^{2}-B^{2}\right)$ with $A=\omega_{c} \sqrt{x}$ and $B=i \omega_{n}+\mu$. Using $D=\left(\omega_{c}^{2} L^{2}\right) /\left(2 \pi v_{F}^{2}\right)$ and further simplifying, we get

$$
\begin{equation*}
\Omega_{\mathrm{osc}}=-\frac{\omega_{c}^{2} L^{2} T}{\pi v_{F}^{2}} \sum_{l=1}^{\infty} \sum_{\omega_{n}} \frac{\omega_{c}^{2}}{2 \pi l} \int_{0}^{\infty} \mathrm{d} x \frac{\sin (2 \pi l x)}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x} \tag{4.2}
\end{equation*}
$$



Figure 4.1: Caption

If we consider only the integral, we have

$$
\begin{equation*}
\int_{0}^{\infty} \mathrm{d} x \frac{\sin (2 \pi l x)}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x}=\frac{1}{2 i} \int_{0}^{\infty} \mathrm{d} x\left\{\frac{e^{i 2 \pi l x}}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x}-\frac{e^{-i 2 \pi l x}}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x}\right\} \tag{4.3}
\end{equation*}
$$

where we used that $2 i \sin (x)=e^{i x}-e^{-i x}$ for the last equality. We can now use contour integration and the Residue theorem to perform the integral, where we use the contours in Fig. 4.1(a) and (b) for the first and and second terms respectively, and we treat ' $x$ ' as a complex number. For the first term in (4.3), we have

$$
\begin{aligned}
2 \pi i \sum_{x_{0}} \operatorname{Res}\left(f, x_{0}\right) & =\int_{a_{1}} \mathrm{~d} x \frac{e^{i 2 \pi l x}}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x}+\int_{b_{1}} \mathrm{~d} x \frac{e^{i 2 \pi l x}}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x} \\
& =\int_{0}^{\infty} \mathrm{d} x \frac{e^{i 2 \pi l x}}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x}+\int_{i \infty}^{0} \mathrm{~d} x \frac{e^{i 2 \pi l x}}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x}
\end{aligned}
$$

where the residues are summed over all poles $x_{0}$ of the integral function $f$, and we note that the path $c_{1}$ vanishes when taken to infinity. We can see that the function has a pole at

$$
x_{0}=\frac{\left(i \omega_{n}+\mu\right)^{2}}{\omega_{c}^{2}}=\frac{-\omega_{n}^{2}+2 i \omega_{n} \mu+\mu^{2}}{\omega_{c}^{2}}
$$

and it lies within the contour if $\omega_{n} \mu \geq 0$ and $\mu^{2}-\omega_{n}^{2} \geq 0$. In this case, the residue is

$$
\operatorname{Res}\left(f, x_{0}\right)=\frac{-1}{\omega_{c}^{2}} e^{i 2 \pi l \frac{\left(i \omega_{n}+\mu\right)^{2}}{\omega_{c}^{2}}}
$$

and hence we get

$$
\begin{align*}
\int_{0}^{\infty} \mathrm{d} x \frac{e^{i 2 \pi l x}}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x}= & -\int_{i \infty}^{0} \mathrm{~d} x \frac{e^{i 2 \pi l x}}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x} \\
& +2 \pi i\left(\frac{-1}{\omega_{c}^{2}}\right) e^{i 2 \pi i \frac{\left(i \omega_{n}+\mu\right)^{2}}{\omega_{c}^{2}}} \Theta\left(\omega_{n} \mu\right) \Theta\left(\mu^{2}-\omega_{n}^{2}\right) \tag{4.4}
\end{align*}
$$

where $\Theta(x)$ is the Heaviside step function that is 1 for $x \geq 0$ and 0 otherwise. The situation is similar for the second integral of (4.3), where the pole is at the same location and the contour $c_{2}$ also vanishes. On the other hand, the winding number of the contour is -1 and must be taken into account. The residue is

$$
\operatorname{Res}\left(f, x_{0}\right)=\frac{-1}{\omega_{c}^{2}} e^{-i 2 \pi l \frac{\left(i \omega_{n}+\mu\right)^{2}}{\omega_{c}^{2}}},
$$

which lies inside the contour only if $\omega_{n} \mu \leq 0$ and $\mu^{2}-\omega_{n}^{2} \geq 0$. Hence, we have

$$
\begin{align*}
\int_{0}^{\infty} \mathrm{d} x \frac{e^{-i 2 \pi l x}}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x}= & -\int_{-i \infty}^{0} \mathrm{~d} x \frac{e^{-i 2 \pi l x}}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x} \\
& +2 \pi i(-1)\left(\frac{-1}{\omega_{c}^{2}}\right) e^{-i 2 \pi i \frac{\left(i \omega_{n}+\mu\right)^{2}}{\omega_{c}^{2}}} \Theta\left(-\omega_{n} \mu\right) \Theta\left(\mu^{2}-\omega_{n}^{2}\right), \tag{4.5}
\end{align*}
$$

and using (4.4) and (4.5), the integral (4.3) is

$$
\begin{aligned}
\int_{0}^{\infty} \mathrm{d} x \frac{\sin (2 \pi l x)}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x}=\frac{1}{2 i}\{ & \int_{0}^{i \infty} \mathrm{~d} x \frac{e^{i 2 \pi l x}}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x}+\int_{-i \infty}^{0} \mathrm{~d} x \frac{e^{-i 2 \pi l x}}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x} \\
& +2 \pi i\left(\frac{-1}{\omega_{c}^{2}}\right) e^{i 2 \pi i \frac{\left(i \omega_{n}+\mu\right)^{2}}{\omega_{c}^{2}}} \Theta\left(\omega_{n} \mu\right) \Theta\left(\mu^{2}-\omega_{n}^{2}\right) \\
& \left.-2 \pi i(-1)\left(\frac{-1}{\omega_{c}^{2}}\right) e^{-i 2 \pi i \frac{\left(i \omega_{n}+\mu\right)^{2}}{\omega_{c}^{2}}} \Theta\left(-\omega_{n} \mu\right) \Theta\left(\mu^{2}-\omega_{n}^{2}\right)\right\}
\end{aligned}
$$

where we switched the limits of the first integral to eliminate the minus sign. With further simplification, we get

$$
\begin{aligned}
\int_{0}^{\infty} \mathrm{d} x \frac{\sin (2 \pi l x)}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x}=-\frac{1}{2}\{ & \left.\int_{0}^{-\infty} \mathrm{d} x^{\prime} \frac{e^{2 \pi l x^{\prime}}}{\left(i \omega_{n}+\mu\right)^{2}+i \omega_{c}^{2} x^{\prime}}+\int_{\infty}^{0} \mathrm{~d} x^{\prime} \frac{e^{-2 \pi l x^{\prime}}}{\left(i \omega_{n}+\mu\right)^{2}+i \omega_{c}^{2} x^{\prime}}\right\} \\
& -\frac{\pi}{\omega^{2}} \Theta\left(\mu^{2}-\omega_{n}^{2}\right)\left[e^{i 2 \pi i \frac{\left(i \omega_{n}+\mu\right)^{2}}{\omega_{c}^{2}}} \Theta\left(\omega_{n} \mu\right)+e^{-i 2 \pi i \frac{\left(i \omega_{n}+\mu\right)^{2}}{\omega_{c}^{2}}} \Theta\left(-\omega_{n} \mu\right)\right]
\end{aligned}
$$

where we substituted $x^{\prime}=i x$ and $\mathrm{d} x^{\prime}=i \mathrm{~d} x$ for the integrals. The limits of integration change from $(i \infty, 0) \rightarrow(-\infty, 0)$ and $(0,-i \infty) \rightarrow(0, \infty)$ for the first and second integral respectively. We can further shift the first integral using $x^{\prime \prime}=-x^{\prime}$ and $\mathrm{d} x^{\prime \prime}=-\mathrm{d} x^{\prime}$, and the limits change from $(-\infty, 0) \rightarrow(\infty, 0)$. For the second integral, we only shift the limits and thus paying a negative sign. Hence, we get

$$
\begin{aligned}
\int_{0}^{\infty} \mathrm{d} x \frac{\sin (2 \pi l x)}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x}=-\frac{1}{2}\{ & \left.-\int_{0}^{\infty} \mathrm{d} x^{\prime \prime} \frac{e^{-2 \pi l x^{\prime \prime}}}{\left(i \omega_{n}+\mu\right)^{2}-i \omega_{c}^{2} x^{\prime \prime}}-\int_{0}^{\infty} \mathrm{d} x^{\prime} \frac{e^{-2 \pi l x^{\prime}}}{\left(i \omega_{n}+\mu\right)^{2}+i \omega_{c}^{2} x^{\prime}}\right\} \\
& -\frac{\pi}{\omega^{2}} \Theta\left(\mu^{2}-\omega_{n}^{2}\right)\left[e^{i 2 \pi i \frac{\left(i \omega_{n}+\mu\right)^{2}}{\omega_{c}^{2}}} \Theta\left(\omega_{n} \mu\right)+e^{-i 2 \pi i \frac{\left(i \omega_{n}+\mu\right)^{2}}{\omega_{c}^{2}}} \Theta\left(-\omega_{n} \mu\right)\right]
\end{aligned}
$$

and renaming all integration variables to $x$ we have

$$
\begin{align*}
\int_{0}^{\infty} \mathrm{d} & \frac{\sin (2 \pi l x)}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x}=\frac{1}{2} \int_{0}^{\infty} \mathrm{d} x e^{-2 \pi l x}\left(\frac{1}{\left(i \omega_{n}+\mu\right)^{2}-i \omega_{c}^{2} x}+\frac{1}{\left(i \omega_{n}+\mu\right)^{2}+i \omega_{c}^{2} x}\right) \\
& -\frac{\pi}{\omega^{2}} \Theta\left(\mu^{2}-\omega_{n}^{2}\right)\left[e^{\frac{-4 \pi \pi \omega_{n} \mu}{\omega_{c}^{2}}} e^{\frac{i 2 \pi l\left(\mu^{2}-\omega_{n}^{2}\right)}{\omega_{c}^{2}}} \Theta\left(\omega_{n} \mu\right)+e^{\frac{4 \pi l \omega_{n} \mu}{\omega_{c}^{2}}} e^{\frac{-i 2 \pi l\left(\mu^{2}-\omega_{n}^{2}\right)}{\omega_{c}^{2}}} \Theta\left(-\omega_{n} \mu\right)\right] \tag{4.6}
\end{align*}
$$



Figure 4.2: a.) Quantum oscillations in the energy (eq.4.7) at $T \in\left\{10^{-1}, 10^{-2}, 10^{-3}\right\}$ at $\mu=1$. b.) Quantum oscillations in the specific heat (eq.4.9) at $T \in\left\{10^{-1}, 10^{-2}, 10^{-3}\right\}$ at $\mu=1$. In both figures, the dashed lines represent the period of the oscillations.

We can now sum both sides over the Matsubara frequencies, as in (4.2), and use that $\sum_{\omega_{n}} f\left(\omega_{n}\right)=$ $\sum_{\omega_{n}>0}\left(f\left(\omega_{n}\right)+f\left(-\omega_{n}\right)\right)$. Hence, we get

$$
\begin{aligned}
\sum_{\omega_{n}} \int_{0}^{\infty} \mathrm{d} & \frac{\sin (2 \pi l x)}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x}=\sum_{\omega_{n}>0}\left(\mu^{2}-\omega_{n}^{2}\right) \int_{0}^{\infty} \mathrm{d} x e^{-2 \pi l x}\left(\frac{1}{\left(\mu^{2}-\omega_{n}^{2}\right)^{2}+\left(2 \omega_{n} \mu-\omega_{c}^{2} x\right)^{2}}\right. \\
& \left.+\frac{1}{\left(\mu^{2}-\omega_{n}^{2}\right)^{2}+\left(2 \omega_{n} \mu+\omega_{c}^{2} x\right)^{2}}\right)-\frac{4 \pi}{\omega_{c}^{2}} \sum_{\omega_{n}>0} \Theta\left(\mu^{2}-\omega_{n}^{2}\right) e^{\frac{-4 \pi l \omega_{n}|\mu|}{\omega_{c}^{2}}} \cos \left(\frac{2 \pi l\left(\mu^{2}-\omega_{n}^{2}\right)}{\omega_{c}^{2}}\right)
\end{aligned}
$$

where for the first term, we used that $1 /(A+B)+1 /(A-B)=2 A /\left(A^{2}-B^{2}\right)$, and for the second term, we used $2 \cos (x)=e^{i x}+e^{-i x}$. The modulus on $\mu$ comes from the fact that $\mu$ has opposite signs for $\Theta\left(\omega_{n} \mu\right)$ and $\Theta\left(-\omega_{n} \mu\right)$. Finally, since the integral does not does contribute to oscillations, we get

$$
\sum_{\omega_{n}} \int_{0}^{\infty} \mathrm{d} x \frac{\sin (2 \pi l x)}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x} \stackrel{\text { osc }}{=}-\frac{4 \pi}{\omega_{c}^{2}} \sum_{\omega_{n}>0} \Theta\left(\mu^{2}-\omega_{n}^{2}\right) e^{\frac{-4 \pi l \omega_{n}|\mu|}{\omega_{c}^{c}}} \cos \left(\frac{2 \pi l\left(\mu^{2}-\omega_{n}^{2}\right)}{\omega_{c}^{2}}\right),
$$

and inserting in (4.2), the final result reads

$$
\begin{equation*}
\Omega_{\mathrm{osc}}=\frac{2 \omega_{c}^{2} L^{2} T}{\pi v_{F}^{2}} \sum_{l=1}^{\infty} \sum_{\omega_{n}>0}^{|\mu|} \frac{1}{l} e^{-\frac{4 \pi l \omega_{n}|\mu|}{\omega_{c}^{2}}} \cos \left(\frac{2 \pi l\left(\mu^{2}-\omega_{n}^{2}\right)}{\omega_{c}^{2}}\right) \tag{4.7}
\end{equation*}
$$

where the upper limit of the Matsubara sum comes from $\Theta\left(\mu^{2}-\omega_{n}^{2}\right)$. We note that the fundamental frequency (when $l=1$ and $n=0$ ) of (4.7) with respect to $\omega_{c}^{-2}$ is $\mu^{2}-\pi^{2} T^{2}$. In the case where $\mu \gg T$, we can neglect the temperature dependence in the cos term in eq. 4.7.

The result of eq. 4.2 is shown in fig. $4.2(\mathrm{a})$ for various temperatures, and illustrates some important features. Firstly, the greater the temperature, the faster the oscillations decrease in amplitude, which makes quantum oscillations at high temperature difficult to detect. The damping effect can be understood by considering the exponential in eq. 4.2, which, for a given $\omega_{c}$ decreases as $T$ increases. Secondly, while the oscillations appear mostly as a sine, they have a cusp-like shape for lower temperatures. This is because the sum over Matsubara frequencies includes more terms as the temperature decreases, giving rise to more harmonics.

### 4.2.1 Specific Heat

The specific heat is related to the grand potential by

$$
\begin{equation*}
c=-T \frac{\partial}{\partial T}\left(\frac{\partial \Omega}{\partial T}\right)_{B} \tag{4.8}
\end{equation*}
$$

and for the oscillatory part of $c$, denoted $c_{\mathrm{osc}}$, we replace $\Omega$ by $\Omega_{\mathrm{osc}}$. Hence, from eq. 4.7, we get

$$
\begin{align*}
c_{\mathrm{osc}}=\frac{8 L^{2}}{v_{F}^{2}} \sum_{l=1}^{\infty} \sum_{\omega_{n}>0}^{|\mu|} \omega_{n} e^{-\frac{4 \pi l \omega_{n}|\mu|}{\omega_{c}^{2}}} & {\left[\cos \left(\frac{2 \pi l\left(\mu^{2}-\omega_{n}^{2}\right)}{\omega_{c}^{2}}\right)\left\{|\mu|\left(2-\frac{4 \pi l|\mu| \omega_{n}}{\omega_{c}^{2}}\right)+\frac{4 \pi l}{\omega_{c}^{2}} \omega_{n}^{3}\right\}\right.} \\
& \left.-\sin \left(\frac{2 \pi l\left(\mu^{2}-\omega_{n}^{2}\right)}{\omega_{c}^{2}}\right)\left\{\omega_{n}\left(3-2 \frac{4 \pi l|\mu| \omega_{n}}{\omega_{c}^{2}}\right)\right\}\right] \tag{4.9}
\end{align*}
$$

Note that technically the sum over the Matsubara frequencies should be performed before differentiating, but this issue was overlooked. In any case, the results of eq. 4.9 are shown in fig $4.2(\mathrm{~b})$. As for the case of $\Omega_{\mathrm{osc}}$, the higher temperatures decay faster and appear to have less harmonics. However, the oscillations are more complex than for $\Omega_{\text {osc }}$, perhaps due to the eq. 4.9 having both sine and cosine terms.

### 4.3 Twisted Bilayer Graphene

We will now derive the Lifshitz-Kosevich (LK) formula for twisted bilayer graphene (TBG), neglecting any disorder or interaction effects, and using the approximation from section 3.2.3. This derivation is similar to that of graphene, and therefore some details will be omitted. The eigenvalues of the inverse non-interacting Green's function are

$$
g_{m, \pm}^{-1}=i \omega_{n}+\mu \pm \omega_{c} \sqrt{m / 4}
$$

The grand potential is then

$$
\begin{aligned}
\Omega_{\mathrm{osc}} & =2 D T \sum_{l=1}^{\infty} \sum_{\omega_{n}} \sum_{\lambda= \pm 1} \int_{0}^{\infty} \mathrm{d} x \frac{1}{i \omega_{n}+\mu+\lambda \omega_{c} \sqrt{x / 4}} \frac{\lambda \omega_{c}}{8 \sqrt{x / 4}} \frac{\sin (2 \pi l x)}{2 \pi l} \\
& =2 D T \sum_{l=1}^{\infty} \sum_{\omega_{n}} \int_{0}^{\infty} \mathrm{d} x \frac{\sin (2 \pi l x)}{2 \pi l} \frac{\omega_{c}}{8 \sqrt{x / 4}} \frac{2 \omega_{c} \sqrt{x / 4}}{\omega_{c}^{2} x / 4-\left(i \omega_{n}+\mu\right)^{2}}
\end{aligned}
$$

where we used a sum over $\lambda$ to account for the ' $\pm$ ' sign. Further simplifying, and using $D=$ $\left(\omega_{c}^{2} L^{2}\right) /\left(2 \pi v_{F}^{2}\right)$, we get

$$
\begin{equation*}
\Omega_{\mathrm{osc}}=-\frac{\omega_{c}^{2} L^{2} T}{4 \pi v_{F}^{2}} \sum_{l=1}^{\infty} \sum_{\omega_{n}} \frac{\omega_{c}^{2}}{2 \pi l} \int_{0}^{\infty} \mathrm{d} x \frac{\sin (2 \pi l x)}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x / 4} \tag{4.10}
\end{equation*}
$$

If we consider only the integral, we have

$$
\begin{equation*}
\int_{0}^{\infty} \mathrm{d} x \frac{\sin (2 \pi l x)}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x / 4}=\frac{1}{2 i} \int_{0}^{\infty} \mathrm{d} x\left\{\frac{e^{i 2 \pi l x}}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x / 4}-\frac{e^{-i 2 \pi l x}}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x / 4}\right\} \tag{4.11}
\end{equation*}
$$

and we can now use contour integration and the Residue theorem to perform the integral, where we proceed is a similar way to the case for graphene, and use the same contours. The first term in the integral has a pole at

$$
x_{0}=\frac{4\left(i \omega_{n}+\mu\right)^{2}}{\omega_{c}^{2}}=\frac{4\left(-\omega_{n}^{2}+2 i \omega_{n} \mu+\mu^{2}\right)}{\omega_{c}^{2}},
$$

which lies within the contour of fig. 4.1(a) if $\omega_{n} \mu \geq 0$ and $\mu^{2}-\omega_{n}^{2} \geq 0$, and the residue is

$$
\operatorname{Res}\left(f, x_{0}\right)=\frac{-4}{\omega_{c}^{2}} e^{i 8 \pi l \frac{\left(i \omega_{n}+\mu\right)^{2}}{\omega_{c}^{2}}}
$$

The second term has a pole at the same location, which lies in the contour of fig. 4.1(b) when $\omega_{n} \mu \leq 0$ and $\mu^{2}-\omega_{n}^{2} \geq 0$, and the residue is

$$
\operatorname{Res}\left(f, x_{0}\right)=\frac{-4}{\omega_{c}^{2}} e^{-i 8 \pi l \frac{\left(i \omega_{n}+\mu\right)^{2}}{\omega_{c}^{2}}}
$$

Hence, inferring from the case for graphene, eq. 4.11 becomes

$$
\begin{aligned}
\int_{0}^{\infty} \mathrm{d} x \frac{\sin (2 \pi l x)}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x / 4}=\frac{1}{2 i}\{ & \int_{0}^{i \infty} \mathrm{~d} x \frac{e^{i 2 \pi l x}}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x / 4}+\int_{-i \infty}^{0} \mathrm{~d} x \frac{e^{-i 2 \pi l x}}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x / 4} \\
& +2 \pi i\left(\frac{-4}{\omega_{c}^{2}}\right) e^{i 8 \pi l \frac{\left(i \omega_{n}+\mu\right)^{2}}{\omega_{c}^{2}}} \Theta\left(\omega_{n} \mu\right) \Theta\left(\mu^{2}-\omega_{n}^{2}\right) \\
& \left.-2 \pi i(-1)\left(\frac{-4}{\omega_{c}^{2}}\right) e^{-i 8 \pi l \frac{\left(i \omega_{n}+\mu\right)^{2}}{\omega_{c}^{2}}} \Theta\left(-\omega_{n} \mu\right) \Theta\left(\mu^{2}-\omega_{n}^{2}\right)\right\}
\end{aligned}
$$

We can neglect the integral terms since they don't contribute to the oscillations, and we get

$$
\int_{0}^{\infty} \mathrm{d} x \frac{\sin (2 \pi l x)}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x / 4}=-\frac{4 \pi}{\omega^{2}} \Theta\left(\mu^{2}-\omega_{n}^{2}\right)\left[e^{i 8 \pi l \frac{\left(i \omega_{n}+\mu\right)^{2}}{\omega_{c}^{2}}} \Theta\left(\omega_{n} \mu\right)+e^{-i 8 \pi l \frac{\left(i \omega_{n}+\mu\right)^{2}}{\omega_{c}^{2}}} \Theta\left(-\omega_{n} \mu\right)\right]
$$

and performing the Matusbara sum as for graphene, we get

$$
\sum_{\omega_{n}} \int_{0}^{\infty} \mathrm{d} x \frac{\sin (2 \pi l x)}{\left(i \omega_{n}+\mu\right)^{2}-\omega_{c}^{2} x / 4}=-\frac{16 \pi}{\omega_{c}^{2}} \sum_{\omega_{n}>0} \Theta\left(\mu^{2}-\omega_{n}^{2}\right) e^{\frac{-16 \pi l \omega_{n}|\mu|}{\omega_{c}^{2}}} \cos \left(\frac{8 \pi l\left(\mu^{2}-\omega_{n}^{2}\right)}{\omega_{c}^{2}}\right)
$$

The final result the reads

$$
\begin{equation*}
\Omega_{\mathrm{osc}}=\frac{2 \omega_{c}^{2} L^{2} T}{\pi v_{F}^{2}} \sum_{l=1}^{\infty} \sum_{\omega_{n}>0}^{|\mu|} \frac{1}{l} e^{\frac{-16 \pi l \omega_{n}|\mu|}{\omega_{c}^{2}}} \cos \left(\frac{8 \pi l\left(\mu^{2}-\omega_{n}^{2}\right)}{\omega_{c}^{2}}\right) \tag{4.12}
\end{equation*}
$$

where the upper limit of the Matsubara sum comes from $\Theta\left(\mu^{2}-\omega_{n}^{2}\right)$. We note that the fundamental frequency (when $l=1$ and $n=0$ ) of (4.7) with respect to $\omega_{c}^{-2}$ is $\mu^{2}-\pi^{2} T^{2}$. Differentiating eq. 4.7 twice w.r.t to T gives us the oscillation in the specific heat

$$
\begin{align*}
c_{\mathrm{osc}}=\frac{8 L^{2}}{v_{F}^{2}} \sum_{l=1}^{\infty} \sum_{\omega_{n}>0}^{|\mu|} \omega_{n} e^{-\frac{4 \pi l \omega_{n}|\mu|}{\omega_{c}^{2}}} & {\left[\cos \left(\frac{2 \pi l\left(\mu^{2}-\omega_{n}^{2}\right)}{\omega_{c}^{2}}\right)\left\{|\mu|\left(2-\frac{4 \pi l|\mu| \omega_{n}}{\omega_{c}^{2}}\right)+\frac{4 \pi l}{\omega_{c}^{2}} \omega_{n}^{3}\right\}\right.} \\
& \left.-\sin \left(\frac{2 \pi l\left(\mu^{2}-\omega_{n}^{2}\right)}{\omega_{c}^{2}}\right)\left\{\omega_{n}\left(3-2 \frac{4 \pi l|\mu| \omega_{n}}{\omega_{c}^{2}}\right)\right\}\right] \tag{4.13}
\end{align*}
$$

## Chapter 5

## Results

From the previous chapter, we have the analytical result for the quantum oscillations, and we now present the numerical results and compare them to the analytical solution. First we mention how we obtain the quantum oscillations from the numerical Landau levels, we then provide an example for graphene, and finally give the results for twisted bilayer graphene (TBG), and discuss their significance.

### 5.1 Method

The numerical results are obtained by using eq. 4.1, where we first perform the Matsubara summation to get

$$
\begin{equation*}
\Omega_{\mathrm{osc}}=T \omega_{c}^{2} \sum_{m=0}^{\infty} G\left(\epsilon_{m}\left(\omega_{c}\right), \mu, \sigma\right) \ln \left(1+e^{-\frac{\epsilon_{m}\left(\omega_{c}\right)-\mu}{T}}\right) \tag{5.1}
\end{equation*}
$$

where $\mu$ is the Fermi energy, $T$ is the temperature, $\epsilon_{m}\left(\omega_{c}\right)$ is the $m^{\text {th }}$ Landau level and we emphasize the fact that $\epsilon$ depends on $\omega_{c}$, and

$$
G(x, \mu, \sigma)=e^{-\frac{(x-\mu)^{2}}{2 \sigma^{2}}}
$$

is a Gaussian function such that $G(\mu, \mu, \sigma)=1$. This function weighs the eigenvalues such that only the eigenvalues close to the Fermi energy contribute to $\Omega_{\mathrm{osc}}$ and therefore the constant background is eliminated. Also note that the only factors kept from eq. 4.1 are $\omega_{c}^{2}$ and $T$. For $T \ll \mu$, we can also use

$$
\begin{equation*}
\Omega_{\mathrm{osc}}=\omega_{c} \sum_{m=0}^{M} G\left(\epsilon_{m}\left(\omega_{c}\right), \mu, \sigma\right)\left(\epsilon_{m}\left(\omega_{c}\right)-\mu\right), \tag{5.2}
\end{equation*}
$$

where $M$ is the largest Landau index for which $\epsilon_{M}<\mu$ is true.
As mentioned in previous sections, at $T=0$, the $n^{\text {th }}$ oscillation is due to the $n^{\text {th }}$ Landau level crossing over the Fermi energy. Since we know the period of the oscillations from the analytical results, we can deduce what magnetic field is required to target oscillations caused by specific Landau levels. For $T \neq 0$, this is still valid, since the effect of finite temperature only blurs the oscillations, and if the temperature is not too high, the period will remain more or less the same. Based on the analytical results, we have noted that the period depend on $\mu$, such that it is in principle possible to target oscillations caused by any Landau level at any magnetic field by fine tuning $\mu$. However,


Figure 5.1: Comparison between the analytical quantum oscillations in energy (eq. 4.7) and the numerical results for $T \in\left\{10^{-5}, 10^{-2}\right\}$ eV, and where the dashed lines represent the period of oscillation as expected from analytical calculations.
there several constraints that we must consider. First of all, high magnetic fields ( $\omega_{c}>0.1$ ) are not achievable experimentally. We will still consider such high magnetic fields, but we will note that such results have little use. Furthermore, low magnetic fields ( $\omega_{c}<0.03$ ) are difficult to obtain numerical results for, and therefore are impractical. Lastly, since our model for TBG is accurate for energies lower than 1 eV , we must require that $\mu<1 \mathrm{eV}$. Again, we will consider higher values of $\mu$, but we will comment on their application.

### 5.2 Results for Graphene

We will now consider the case of graphene, as to test our numerical method with the analytical results. The numerical results for graphene are shown in Fig. 5.1 for $T=10^{-5}$ and $=10^{-2} \mathrm{eV}$, with $\mu=1$ and $\sigma=1$, and the analytical results are provided for comparison. The numerical values were diagonalized using the numerical method established in section 3 , while the analytical solution is taken from eq. 4.7. The range of magnetic fields probed is $\omega_{c}=1$ to $\omega_{c}=0.01$, which corresponds to $B=\sim 10^{3} \mathrm{~T}$ and $B \sim 0.1 \mathrm{~T}$. The numerical results for the specific heat are not shown since they are expected to be identical to the analytical results from Fig. 4.1. As we can see, the numerical results agree with the analytical results, up to an overall factor, which we have neglected. In any case, the period of oscillation identical, as well as the effect of temperature.

### 5.3 Results for Twisted Bilayer Graphene

The numerical results for TBG are shown in Fig. 5.2, for $T=10^{-4} \mathrm{eV}$, for $\theta \in\left\{1.05^{\circ}, 5.00^{\circ}\right\}$, and $\mu \in\{7.07 \mathrm{eV}, 10 \mathrm{eV}\}$. The results were generated for magnetic fields around $\omega_{c} \sim 1$, which corresponds to oscillations caused by the $200^{\text {th }}$ and $400^{\text {th }}$ Landau level for $\mu=7.07 \mathrm{eV}$ and $\mu=10.0$ eV respectively. The cutoffs used were $N=200$ and $N=300$ for $\mu=7.07 \mathrm{eV}$ and $\mu=10.0$, and we have used $\sigma=1$. The vertical dashed lines show the expected period obtained from the analytical solution from eq. 4.12 , which is $4\left(\mu^{2}-\pi^{2} T^{2}\right)$, precisely 4 times smaller than the period for graphene


Figure 5.2: Numerical quantum oscillations for $T B G$ at $T=10^{-4}$ eV ( $\sim 1^{\circ} \mathrm{K}$ ), where oscillations for $\mu=7.07 \mathrm{eV}$ and $\mu=10 \mathrm{eV}$ correspond to oscillations around the $200^{\text {th }}$ and $400^{\text {th }}$ Landau level. The oscillations were calculated around $\omega_{c}^{2} \sim 1$ ( $\sim 900$ Teslas), and the y-axis is arbitrary, since we have neglected an overall constant factor.
oscillations. As previously noted, these results have been obtained for values of $\omega_{c}$ and $\mu$ that do not correspond to situations that have physical use. Nevertheless, we shall still interpret them.

First of all, in fig. $5.2(\mathrm{a})$ and (b), we note that for $1.00 \lesssim \omega_{c} \lesssim 1.06$ (for (a)) and $1.00 \lesssim$ $\omega_{c} \lesssim 1.03$ (for (b)), the oscillations correspond somewhat to the analytical prediction. However, for $1.08 \lesssim \omega_{c} \lesssim 1.20$ (for (a)) and $1.04 \lesssim \omega_{c} \lesssim 1.10$ (for (b)), oscillations with a lower frequency appears. From the figure, one can deduce that the frequency is 4 times greater than the analytical prediction, and coincides with the frequency for graphene oscillations. As noted in subsection 3.2.3, the analytical approximation agrees well with results around $\omega_{c} \sim 0.1$, so this behaviour is somewhat unexpected. A possible reason for this is due to the fact that the magnetic field used is high. In such case, the diagonal terms in the TBG Hamiltonian are significantly larger than the off diagonal terms, in which case the spectrum resembles that of graphene. For the case of fig. 5.2(c) and (d), the oscillations agree more with the analytical results. There is still a region where oscillations with a lower frequency appear, but they are less prominent than in fig. 5.2(c) and (d).

Fig. 5.3 shows the results for same values of $\mu, \omega$ and $\theta$, but at higher temperatures, namely $T \in\left\{10^{-3}, 10^{-2}\right\} \mathrm{eV}$. The cutoffs used were $N=200$ and $N=300$ again for $\mu=7.07 \mathrm{eV}$ and


Figure 5.3: Numerical quantum oscillations for TBG at $T \in\left\{10^{-3}, 10^{-2}\right\}$ eV ( $\sim 10^{\circ} \mathrm{K}$ and $100^{\circ} \mathrm{K}$ ), where oscillations for $\mu=7.07 \mathrm{eV}$ and $\mu=10 \mathrm{eV}$ correspond to oscillations around the $200^{\text {th }}$ and $400^{\text {th }}$ Landau level. The oscillations were calculated around $\omega_{c}^{2} \sim 1(\sim 900$ Teslas $)$, and the $y$-axis is arbitrary, since we have neglected an overall constant factor.
$\mu=10.0$, and we have used $\sigma=1$. As expected, for higher temperatures, the oscillations have lower amplitude, and the high frequency harmonics get significantly damped. Hence, in all cases, at $T=10^{-3} \mathrm{eV}$, the oscillations predicted analytically (i.e the oscillations with period similar to the vertical dashed lines) are still observable, but vanish at $T=10^{-2} \mathrm{eV}$. On the other hand, lower frequency oscillations are still observable up to temperatures of $T=10^{-2} \mathrm{eV}$.

Fig. 5.4 shows the results for $T=10^{-5} \mathrm{eV}$, for $\theta \in\left\{1.05^{\circ}, 5.00^{\circ}\right\}$, and $\mu=0.707 \mathrm{eV}$. For such $\mu$, the model is expected to produce physically meaningful results. The results were generated for magnetic fields around $\omega_{c} \sim 0.1$, which corresponds to oscillations caused by the $200^{\text {th }}$ Landau level for $\mu=0.707 \mathrm{eV}$. Such magnetic fields correspond to $\sim 9$ Teslas, which is a reasonable value for experiments. Furthermore, note that the temperature is a full order of magnitude lower than in fig. 5.2 , since the magnetic field is now lower. The cutoff used was $N=400$, and we have used $\sigma=0.05$.

One striking difference between fig. $5.4(\mathrm{a})$ and (b) is the presence of clear lower frequency oscillations for (b) but not for (a). The period for the lower frequency oscillation in (b) is $\sim 18$ times larger than the predicted TBG period, shown by the dashed vertical lines. At this regime, the model is expected to give realistic results, and therefore such oscillations should not in principle


Figure 5.4: Numerical quantum oscillations for TBG at $T=10^{-5} \mathrm{eV}\left(\sim 0.1^{\circ} \mathrm{K}\right)$, where oscillations for $\mu=0.707 \mathrm{eV}$ correspond to oscillations around the $200^{\text {th }}$ Landau level. The oscillations were calculated around $\omega_{c}^{2} \sim 0.1(\sim 9$ Teslas), and the $y$-axis is arbitrary, since we have neglected an overall constant factor.
be an artifact of the Hamiltonian from eq. 1.8. Nevertheless, the frequency of this oscillation does not coincide with any prediction. The second striking difference between fig. $5.4(\mathrm{a})$ and (b) is the complete lack of agreement of (a) with the analytical prediction, while (b) agrees well, especially at the valleys of the low frequency oscillation. This could be because at $\theta=1.05^{\circ}$, the Dirac cone picture is not justified anymore, and the analytical approximation is characteristic of a Dirac cone. In any case, the results for $\theta=1.05^{\circ}$ (i.e. (a)) are problematic due to the onset of Landau level splitting at such angles[19]. For high magnetic fields, the Landau level spectrum is expected to split, where the specific magnetic field at which this happens is lower if the real space unit cell is larger. For $\theta=1.05^{\circ}$, the onset of Landau level splitting[22] is $\sim 3$ Teslas, while for $\theta=5.00^{\circ}$, the onset is $\sim 80$ Teslas. Hence, for $\theta=1.05^{\circ}$, we are clearly in a regime in which Landau level splitting must be considered, but this is not the case for $\theta=5.00^{\circ}$.

Fig. 5.5 shows the results for same value of $\mu, \omega$ and $\theta$, but at higher temperatures, namely $T \in\left\{10^{-4}, 10^{-3}\right\} \mathrm{eV}$. The cutoff used was $N=400$ again, and we have used $\sigma=0.05$. Again, for higher temperatures, the oscillations have lower amplitude, and the high frequency harmonics get significantly damped.


Figure 5.5: Numerical quantum oscillations for $T B G$ at $T \in\left\{10^{-4}, 10^{-3}\right\} e V\left(\sim 1^{\circ} K\right.$ and $\left.10^{\circ} \mathrm{K}\right)$, where oscillations for $\mu=0.707 \mathrm{eV}$ correspond to oscillations around the $200^{\text {th }}$ Landau level. The oscillations were calculated around $\omega_{c}^{2} \sim 0.1$ ( $\sim 9$ Teslas), and the $y$-axis is arbitrary, since we have neglected an overall constant factor.

## Conclusion and Outlook

In this thesis, we have obtained the energy spectrum of twisted bilayer graphene (TBG) numerically using the model from ref. [2], from which we made an analytical approximation. We then derived the quantum oscillations analytically using the Lifshitz-Kosevich and the analytical approximation. Finally, we obtained the quantum oscillations numerically, and compared the results with the analytical derivation. Although most of the results obtained do not lead to realistic cases, some results do indeed describe situations that are possible in experiments. Such results are mainly for $\theta \in\left\{1.05^{\circ}, 5.00^{\circ}\right\}$, for $\omega_{c}=0.1$ ( $\sim 9$ Teslas), and for temeratures of $T \in\left\{10^{-5}, 10^{-4}, 10^{-3}\right\} \mathrm{eV}$ (corresponding to $0.1,1$ and 10 Kelvins respectively). The case for $\theta=1.05^{\circ}$ should not be considered seriously since at such angles, and at such magnetic fields, the Landau levels should split, and this was not taken into account.

For future work, it would be interesting to consider the effect of Landau level splitting. Since at low angles, TBG exhibits a large real space unit cell, it would then be possible to observe the Landau level splitting with magnetic fields that are possible in experiments, and for that reason this is a topic of interest. The authors from ref. [3] use the same model we have used and numerically obtain the fractal structure expected from Landau level splitting, also called the Hofstadter butterfly. Ref. [12] consider a similar model and show that the resulting butterfly has a different nature whether the angle is above or below the first magic angle.

Also to consider, is the physics of TBG at low angles, i.e. angles below $1.05^{\circ}$. At this regime, our model does not produce physical results, although this is precisely where the interesting physics lies, since it is at this range of angles that the model becomes can be superconductive. No analytical model was found for TBG below $1.05^{\circ}$, and numerical computations are costly due to the large number of atoms per TBG unit cell. Recently however, ref. [34] claims to have analytically derived the series of magic angles, which up to now was done only numerically. They have achieved this by considering a chiral model, and their research would be interesting to consider moving forwards.

In the search for flat bands, twisted double bilayer graphene (TDBG) was also considered[17, 31]. This material consists of replacing the graphene sheets in TBG by bilayer graphene. The idea is to use the displacement between the two graphene sheets within a bilayer to further fine tune the onset of superconductivity, along with the twist angle. According to the experiments from ref. $[17,31]$, such has superconductive states at temperatures up to $T=12^{\circ}$ Kelvin, and a theoretical Hamiltonian is provided by [31]. In both papers, quantum oscillations are measured experimentally, thus showing their importance. Given that the numerical scheme developed in this thesis can be applied to any Hamiltonian, it could be interesting to apply it to the model given in [31] for further work.

## Chapter 6

## Appendicies

### 6.1 Appendix A: Poisson Summation

For an arbitrary function $f(n)$ summed over $n$ from $-\infty$ to $\infty$, we have

$$
\sum_{n=-\infty}^{\infty} f(n)=\sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{d} x f(x) \delta(x-n)=\int_{-\infty}^{\infty} \mathrm{d} x f(x) \sum_{n=-\infty}^{\infty} \delta(x-n)
$$

where $\delta(x)$ is the Dirac delta. The first step is due to the Dirac delta's translation property, and in the second step we only moved the sum inside the integral. The term $\sum_{n} \delta(x-n)$ is called a Dirac comb, where its Fourier series is

$$
\sum_{n=-\infty}^{\infty} \delta(x-n)=\sum_{k=-\infty}^{\infty} e^{i 2 \pi k x}
$$

and therefore we get

$$
\sum_{n=-\infty}^{\infty} f(n)=\int_{-\infty}^{\infty} \mathrm{d} x f(x) \sum_{k=-\infty}^{\infty} e^{i 2 \pi k x}
$$

In our case however, the function $f(n)$ is summed over $n$ from 0 to $\infty$, such that we have

$$
\sum_{n=0}^{\infty} f(n)=\lim _{\epsilon \rightarrow 0^{+}} \int_{-\epsilon}^{\infty} \mathrm{d} x f(x) \sum_{n=-\infty}^{\infty} \delta(x-n)=\int_{0}^{\infty} \mathrm{d} x f(x) \sum_{k=-\infty}^{\infty} e^{i 2 \pi k x},
$$

where the integration limit allows us to take the sum of $n$ from $-\infty$ to $\infty$ in the first step, and the lower integration limit must be $\epsilon \rightarrow 0^{+}$to include the $n=0$ term.

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[^0]:    ${ }^{1}$ Since $\boldsymbol{v}$ is the derivative of energy, it points in the direction of energy change, and therefore normal to a surface of constant energy.

[^1]:    ${ }^{1}$ The spectrum is symmetric.

