Electronic and Thermal Properties of Quasi-Free Non-Relativistic And Ultra-Relativistic Electrons

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CERTIFICATE

It is certified that the work contained in this dissertation was carried out by ***Muhammad Irfan Sarwar*** under my supervision and is accepted by the Department of Physics, Quaid-i-Azam University Islamabad as satisfying the dissertation requirement for the degree of Master of Philosophy in Physics.

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Dedicated

To

MY SWEET PARENTS

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All prays and glory is due to ALLAH, Whose worth cannot be described even by the greatest rhetoricians of all times, Whose blessings and bounties cannot be enumerated by beckoners and enumerators of all ages, and homage due to Him cannot be adequately paid even by the most assiduous and revering attempters.

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ABSTRACT

The purpose of this work is to provide a brief description of the transport of the particles and heat energy in the non-relativistic and ultra-relativistic 2DEG in the low temperature limit where linear response theory works. A viable basis of the Landauer theory will be provided to understand the transport of the non-relativistic and ultra-relativistic quasi-free particles and energy. The electrical conductance and thermal conductance quantum will be found by using Landauer theory. This also provides a gateway to find Seebeck and Peltier coefficient. Moreover, we examine the behavior of a 2DEG that is subjected to both a perpendicular magnetic field and spatially varying internal electric fields. We choose one of the two guiding centre to be diagonal. This makes energy a local function of the position, allowing for an easy visualization of the transverse response to externally imposed fields, as well as the spatial distribution of the (transverse) Hall current inside the sample. Further, in this model, we apply a thermal gradient which results into the quantized thermal current flowing through the sample.

Chapter 1

Introduction

Solids are typically classified into three categories depending on their electrical properties: conductors, insulators and semiconductors. Conductors such as metals conduct current well, whereas insulators do not conduct current. The conductivity of semiconductors lie somewhere in between metals and insulators. The current in solids is carried by the electrons, which are elementary particles that behave as both particles and waves. The differences in the electrical properties of solids arise from the interactions between the crystal structures of materials and electrons. In solids, this interaction will give rise to an energy gap in the allowed states of electrons in the material. In semiconductors and insulators, the energy gap divides electrons into bound electrons, the so-called conduction band electrons. How well a semiconductor or insulator conducts current, i.e., its conductivity, is related to the number of electrons in the conduction band. In semiconductors the energy gap is large as compare to conductors. This means that semiconductors can conduct fairly well at room temperature since bound electrons can become free mobile charge carriers through thermal excitation. The conductivity of semiconductors can be fine tuned, from metal like to insulating, by introducing so-called doping that can control the number of free carriers in the conduction band, or by using an electric field to shape the band structure.

As the size of the devices become closer to the wavelength of the electrons in the material, a confinement effect will lead to electrons exhibiting low dimension properties. A low dimension system is created when electrons in a conductor are physically confined so that they can no longer move in fully three dimensional space, but only in two dimension, one dimensional or even zero dimensional regions of space. The electronic and thermal properties of low dimensional systems have been the subject of much interest in the last two decades, driven by the twin

goals of discovering new physics and developing potential applications. Studies of low dimensional systems have indeed yielded exciting new discoveries, such as quantum Hall effects, which will be discussed in the coming chapters, for which two Nobel Prizes have been awarded. The electronic properties of low dimensional system remain an important topic of research with ongoing exploration of physical systems. Low-dimensional properties of electrons are clearly seen in two-dimensional electron gases (2DEG) based on semiconductor heterostructures[1].

This thesis is about the electronic and thermal properties of a two dimensional electron gas, confined in a rectangular geometry and subjected to a strong perpendicular magnetic field, in low dimension. We will focus on intellectual curiosities that 2DEG has to offer and, in particular, will discuss several phenomenon that can be observed in electronic and thermal transport.

1.1 Two dimensional electron gas

Many important developments in transport properties have taken place in the two-dimensional electron gas (2DEG), and are likely to continue to do so in the future. We make explicit here the certain approximations with which we shall work. Although transport in semiconductors can be mediated by both electron and hole flow, it is usually just the electrons that are involved. The two-dimensional samples are usually degenerate, which means that the conduction band is highly populated with electrons. Furthermore, transport energy scales are low cf. the band gap and therefore inter-band transitions are avoided. Thus, we need to consider only a single band, the conduction band (CB) and the electrons that reside in it. We consider the electrons to be non-interacting. The justification of non-interacting electron comes from the Fermi gas theory. Fermi gas, or free electron gas, is a physical model assuming a collection of non-interacting fermions. It is the quantum mechanical version of an ideal gas for the case of fermionic particles. Electrons in metals and semiconductors can be approximately considered Fermi gases.

The energy distribution of the fermions in a Fermi gas in thermal equilibrium is determined by their density, temperature, and the set of available energy states, via Fermi-Dirac statistics. By the Pauli principle, no quantum state can be occupied by more than one fermion, so the total energy of the Fermi gas at zero temperature is larger than the product of the number of particles and the single-particle ground state energy. For this reason, the pressure of a Fermi gas is

non-zero even at zero temperature, in contrast to that of a classical ideal gas. It is possible to define a Fermi temperature below which the gas can be considered degenerate. This temperature depends on the mass of the fermions and the energy density of states. For metals, the electron gas Fermi temperature is generally many thousands of kelvins, so they can be considered degenerate. The maximum energy of the fermions at zero temperature is called the Fermi energy. The Fermi energy surface in the momentum space is known as the Fermi surface. Since interactions are neglected by definition, the problem of treating the equilibrium properties and dynamical behaviour of a Fermi gas reduces to the study of the behaviour of a single independent particle. As such, it is still relatively tractable and forms the starting point for more advanced theories (such as Fermi liquid theory in the interaction) which take into account interactions to some degree of accuracy[2].

Another strict justification of free electron gas comes from the Landau theory, in which an interacting electron gas is re-described in terms of non-interacting quasi-particles with renormalised energy (as compared to original particles) and a finite lifetime. Provided this lifetime is long compared to any experimentally relevant processes, the quasi-particle picture is a valid one, and this is generally the case in semiconductors.

1.2 Outline

The rest of this thesis will present a review of the local electronic and thermal properties of 2DEG in the quantum Hall regime and in nano-structures.

In chapter 2, we give a quick review of the classical Drude's theory and use this model of transport to study the electrical and thermal conductivity and the Seebeck coefficient. Then we formulate the semi-classical Boltzmann theory of transport in bulk materials in order to become familiar with some concepts and language, and also have a cachet with which to compare. At the end of this chapter we give a review of Landau theory and mesoscopic transport concepts which are frequently used to calculate the current in the next chapters.

In chapter 3, we present Landau levels to understand the Integer Quantum Hall Effect in a 2DEG. We solve the Schrdinger equation for single particle wave functions and energy spectrum in the symmetric and Landau gauges. Then, we use Landau theory to study the edge currents and conductivity. The

effect of the periodic potential is also introduced in chapter 3 to study the gauge invariance of the Hall conductance. Here, in this chapter we show that the Hall conductance is shown to be represented by a gauge invariant quantity which is naturally an integer.

This is similar to the Laughlin's argument[8] that an exact quantization must be a consequences of a general principle which is determined by the geometrical nature of the problem. Chapter 3 then follows an alternative frame work for a 2DEG. In this section we study the effect of a random confinement potential in a rectangular geometry. We check here that how the Landau levels are modified by introducing this random potential. Then we calculate thermal conductivity in linear response theory by using the Landau formalism.

Chapter 4 introduces graphene, a two dimensional material composed of carbon arranged in a hexagonal lattice. Graphene was first discovered in 2004[15], and in the few years since, it has attracted the attention of researchers. The first thing will come in mind when the physicist hear the word graphene is the linear dispersion relation of the charge carrier.

The low energy properties of the graphene are predicted to be governed by a two dimensional massless Dirac equation[19, 21, 22]. This has confirmed by experiments[23]. The basic properties of Dirac equation are not discussed here, and refer a book such as in [20]. We will go through the derivation of the Dirac Hamiltonian of graphene and go into the more details of the origin of pseudo-spin.

The most striking transport prediction for Dirac electrons is Klein tunneling[9, 10, 15] in the ultra relativistic limit. Imagine a system where a Dirac particle of energy ϵ is in a mono atomic potential which only depends upon x. Suppose it satisfies $U(x \to -\infty) = U_1, U(x \to +\infty) = U_2$, where $U_1 < \epsilon < U_2$, in such configuration a Dirac particle incident normally will be fully transmitted, independent of ϵ. We will explore Klein tunnelling in more detail in chapter 4. This problem will be tackled by using so-called mass confinement. Then, by using this hypothetical mass term, we discuss quantum transport through a constriction which is a counter-part of the derivation which we did before for the non-relativistic case in chapter 2. Finally, we find transport coefficients in terms of transmission probabilities.

Chapter 2

Basic principles

2.1 History

Quantum Hall Effect is a study of the 2D electron gas in a perpendicular magnetic field. It is one of the most interesting topics in the field of research in condensed matter physics. The Quantum Hall Effect is the quantum version of the classical Hall Effect in which conductivity takes discrete values,

$$\sigma = \nu \frac{e^2}{h} \tag{2.1}$$

where e is electron charge and h is Planck's constant and ν is called filling factor. It takes either integer ($\nu = 1, 2, 3.....$) or fractional ($\nu = \frac{1}{3}, \frac{2}{3}, \frac{1}{5}.....$) values. The Quantum Hall Effect is Integer or Fractional Quantum Hall Effect depending on whether the value of ν is integer or fraction respectively. It is well understood in terms of a single electron subjected to a perpendicular magnetic field. The FQHE is somewhat complicated. It involves electron-electron interactions.

The IQHE was first predicted by Ando, Matsumoto, and Uemura in 1975 but they were not sure about the truth of the result which they derived on the basis of approximate calculation. In several experiments this effect is observed, which are carried out on the MOSFET inversion layer. It was Klaus von Klitzing[17] who, first working with Michael Pepper and Gerhard Dorda, experimentally observed the exact quantization of conductivity in 1980. On that marvelous work Von Klitzing was awarded the Nobel Prize in 1985. The connection between exact quantization of conductivity and gauge invariance was developed by Laughlin[8].

2.2 Classical Hall Effect

The conductivity and resistivity tensors can be found using the classical Drude Model. Drude equation of motion is,

$$-\frac{\vec{p}}{\tau}+\vec{F}=\frac{d\vec{p}}{dt}. \tag{2.2}$$

In the steady state,

$$\frac{d\vec{p}}{dt}=0. \tag{2.3}$$

Hence,

$$\vec{F}=\frac{\vec{p}}{\tau} \tag{2.4}$$

and,

$$\vec{v}=\frac{\tau}{m}\vec{F}. \tag{2.5}$$

For the Hall effect in the presence of a magnetic field, the Lorentz force is,

$$\vec{F}=-e\vec{E}-e\left(\frac{\vec{v}\times\vec{B}}{c}\right). \tag{2.6}$$

Resolving the velocity into its components along x and y-direction, and solving for velocity we get

$$-\frac{m}{e\tau}\begin{pmatrix}1 & \omega_c\tau\\ -\omega_c\tau & 1\end{pmatrix}\begin{pmatrix}v_x\\ v_y\end{pmatrix}=\begin{pmatrix}E_x\\ E_y\end{pmatrix}, \tag{2.7}$$

where ω_c is cyclotron frequency of electrons. The current is related with the velocity as

$$\vec{v}=-\frac{\vec{j}}{en}, \tag{2.8}$$

where e is electron charge and n is electron number density so,

$$\frac{m}{ne^2\tau}\begin{pmatrix}1 & \omega_c\tau\\ -\omega_c\tau & 1\end{pmatrix}\begin{pmatrix}j_x\\ j_y\end{pmatrix}=\begin{pmatrix}E_x\\ E_y\end{pmatrix}, \tag{2.9}$$

$$\rho=\frac{1}{\sigma_0}\begin{pmatrix}1 & \omega_c\tau\\ -\omega_c\tau & 1\end{pmatrix},\quad \sigma_0=\frac{ne^2\tau}{m},\quad \rho_{xx}=\frac{1}{\omega_0}=\frac{m}{ne^2\tau},\quad \rho_{xy}=\frac{\omega_c\tau}{\sigma_0}=\frac{B}{nec}, \tag{2.10}$$

$$\rho^{-1} = \sigma = \frac{\sigma_0}{1 + (\omega_c \tau)^2} \begin{pmatrix} 1 & -\omega_c \tau \\ \omega_c \tau & 1 \end{pmatrix}. \tag{2.11}$$

Here is a point to be noted: when $B = 0$, $\sigma_{xy} = 0$. This implies that ρ is diagonal and $\rho_{xx} = \frac{1}{\sigma_{xx}}$. If we have a system where $\sigma_{xx} = 0$, then $\rho_{xx} \to \infty$ and the system is insulator with infinite resistivity. The system is dissipative and joule heating is large. If we have a system where a magnetic field is present, $\sigma_{xy} \neq 0$, $\rho_{xx} \neq \frac{1}{\sigma_{xx}}$. If we have $\sigma_{xx} = 0$, then $\rho_{xx} = 0$, not infinity.

If electron scattering is absent then $\tau \to \infty$ and we have $\rho_{xx} = \sigma_{xx} = 0$, $\rho_{xy} = \frac{B}{nec}$, and we have dissipation-less state with $\vec{j} \perp \vec{E}$. In QHE we find that at certain discrete values of B,

$$\sigma_{xx} = \rho_{xx} = 0, \tag{2.12}$$

$$\sigma_{xy} = \frac{1}{\rho_{xy}} = \nu \frac{e^2}{h}. \tag{2.13}$$

2.3 Thermal conductivity

If we have two systems at different temperatures heat will flow from the hot body to the cold body to attain thermal equilibrium. Heat flux can be calculated by using Fourier's Law $\mathbf{J} = -\kappa \nabla T$, where ∇T is gradient of temperature , J is heat flux, and κ is thermal conductivity. κ is temperature dependent and a scalar if the system is isotropic. Else it is tensor valued.

To understand thermal conductivity we need to start from the atomic level where phonon interactions play an important role in thermal transport. In insulators, heat is carried by the harmonic oscillations of phonons and in metals electrons also play an important rule. Theoretically, for an infinite crystal the thermal conductivity is infinite. But the thermal conductivity of common crystal is finite. There are three main reason for the finite result of the thermal conductivity. Firstly, the scattering from impurities reduced the thermal conductivity. Secondly, the material is finite. Finally, an-harmonic oscillations or umklapp processes are essential for the finite thermal conductivity.

2.3.1 Classical Treatment

In the classical treatment of thermal transport, we use the Drude Model. This was the first attempt made by Paul Drude, to theoretically understand electronic transport properties. Drude assumed that the electrons are free, non-interacting particles carrying heat current as well as electronic current. One finds the electronic conductivity,

$$\sigma = \frac{ne^2}{m}\tau. \tag{2.14}$$

Now apply a thermal gradient across the metal. A thermal current j^s will flow through the metal. From thermodynamics,

$$d\varepsilon = Tds - pdv. \tag{2.15}$$

For a fixed volume,

$$d\varepsilon = dQ = Tds. \tag{2.16}$$

Consider the energy flowing through the plane perpendicular to ∇T and assumes that ∇T is along the x-direction,

$$\vec{\nabla} T = \frac{dT}{dx}\hat{x}. \tag{2.17}$$

Electrons crossing through the planes from left to right have had their last collision, on average, at time τ earlier at the position, $x^L = x - v_x^L\tau$. Here v_x^L is the average speed of these electrons in the x-direction. These electrons have average energies, $\varepsilon\left(T(x - v_x^L\tau)\right)$, where $\varepsilon(T)$ is average energy at temperature T.

Similarly, the electrons moving from right to left have had their last collision at the position, $x^R = x + v_x^R\tau$ and carry average energy, $\varepsilon\left(T(x + v_x^R\tau)\right)$. The number of electrons per unit area per unit time crossing from left to right are,

$$\frac{1}{2}nv_x^R \tag{2.18}$$

and the number of electrons per unit area per unit time crossing from right to left are,

$$\frac{1}{2}nv_x^L. \tag{2.19}$$

The energy flux can be written as,

$$j^q = \frac{1}{2}nv_x^L\varepsilon\left(T(x - v_x^L\tau)\right) - \frac{1}{2}nv_x^R\varepsilon\left(T(x + v_x^R\tau)\right). \tag{2.20}$$

For slow variation of temperature, $\frac{dT}{dx} < \frac{T_0}{\ell}$, where T_0 is average temperature and ℓ is mean free path, we can expand equation (2.20) to get,

$$j^q = \frac{1}{2} n v_x^L \left(\varepsilon\left(T(x)\right) - v_x^L \tau \frac{d\varepsilon}{dT} \times \frac{dT}{dx} \right) - \frac{1}{2} n v_x^R \left(\varepsilon\left(T(x)\right) + v_x^R \tau \frac{d\varepsilon}{dT} \times \frac{dT}{dx} \right). \tag{2.21}$$

By rearranging the above equation we get,

$$j^q = -\frac{1}{2}\tau \frac{d\varepsilon}{dT} \times \frac{dT}{dx} \left[\left(v_x^L\right)^2 + \left(v_x^R\right)^2 \right] + \frac{1}{2} m\varepsilon\left(T(x)\right)\left(v_x^L - v_x^R\right). \tag{2.22}$$

The first term of the equation (2.22) can be approximated as,

$$\frac{1}{2}\left(v_x^L\right)^2 + \frac{1}{2}\left(v_x^R\right)^2 = \langle v_x^2 \rangle = \frac{1}{3}\langle v^2 \rangle = \frac{1}{3}\frac{3k_B T}{m} = \frac{k_B T}{m}. \tag{2.23}$$

In the second term, $v_x^L - v_x^R = \langle v_x \rangle$ is average velocity at position x. But since the thermal conductivity is usually measured in an open circuit, no current will flow in the x-direction. Hence, $\langle v_x \rangle = 0$. Thus, the second term in the equation (2.22) vanishes. We will discuss this point later in this section,

$$j^q = -\frac{1}{3} n\tau \langle v^2 \rangle \frac{d\varepsilon}{dT}\frac{dT}{dx}. \tag{2.24}$$

By the definition of thermal conductivity one reads,

$$\kappa = \frac{1}{3} n\tau \langle v^2 \rangle \frac{d\varepsilon(T)}{dT}, \tag{2.25}$$

where $\varepsilon(T)$ is average energy per electron at temperature T, $N\varepsilon$ is total average energy and $n\varepsilon$ is average energy density. If c_V is specific heat capacity per unit volume at constant volume then,

$$c_V = n\frac{d\varepsilon}{dT} = \frac{3}{2} n k_B. \tag{2.26}$$

Thermal conductivity in equation (2.25) is,

$$\kappa = \frac{1}{3}\langle v^2 \rangle \tau c_V. \tag{2.27}$$

The ratio between the thermal conductivity and electrical conductivity reads,

$$\frac{\kappa}{\sigma} = \left(\frac{3}{2}\frac{k_B^2}{e^2} \right) T = L_0 T. \tag{2.28}$$

Which is the well-known Wiedmann-Franz law. Here $L_0 = \left(\frac{3}{2}\frac{k_B^2}{e^2}\right)$ is Lorentz number, the value of which is 1.11×10^{-8}watt.ohm/k. This is in excellent agreement with the experimental value. This success is just luck. We will see that when we treat electron gas quantum mechanically, the value of $\langle v^2 \rangle$ is greater than 100 times as calculated in the classical case by the Drude's model but the value of c_V is almost 100 times less than the previously calculated value. These two effects exactly cancel each other. So accidentally the Drude model exactly matches the experimental value.

Even in Drude's day, it was known that something is not right since no electronic contribution to specific heat capacity was ever found as large as $\frac{3}{2}nk_B$.

2.3.2 Thermo-electric effect

We state in the previous section, $v_x^L - v_x^R = \langle v \rangle = 0$ in an open circuit. But since, $T(x_L) > T(x_R)$ one would expect that $v_x^L > v_x^R$.

This implies that in the steady state an electric field must generated in the same direction as $\vec{\nabla}T$ that exactly compensates for the difference in thermal velocities so that velocities of right going and left going electrons are equal as they cross the same plane at x.

This is the thermo-electric field $\vec{E}$ and it is proportional to the $\vec{\nabla}T$. We define thermo-power S by the equation

$$\vec{E} = S\vec{\nabla}T. \tag{2.29}$$

We estimate the value of S here. Suppose, $v_{x_0}^L$ is velocity from equilibrium thermal distribution at $T(x - v_x\tau)$, and $v_{x_0}^R$ is velocity from equilibrium thermal distribution at $T(x + v_x\tau)$. When the thermo-electric field $\vec{E}$ is present, the speed of right going electrons when they cross the plane at x is,

$$v_x^L = v_{x_0}^L - \frac{eE\tau}{m} \tag{2.30}$$

Here, $\frac{eE}{m}$ is acceleration due to the presence of electric field. Similarly,

$$v_x^R = v_{x_0}^R + \frac{eE\tau}{m}. \tag{2.31}$$

The temperature dependence of thermal velocities one reads,

$$v_{x_0}^L = v_x\left(T(x - v_x\tau)\right) = v_x\left(T(x)\right) - \frac{dv_x}{dT}.\frac{dT}{dx}v_x\tau, \tag{2.32}$$

$$v_{x_0}^R = v_x\left(T(x + v_x\tau)\right) = v_x\left(T(x)\right) + \frac{dv_x}{dT}.\frac{dT}{dx}v_x\tau \tag{2.33}$$

The difference in velocities must vanish at x. So,

$$\begin{aligned}
&v_x^L - v_x^R = 0,\\
&v_{x_0}^L - \frac{eE\tau}{m} - v_{x_0}^R - \frac{eE\tau}{m} = 0,\\
&v_x\left(T(x)\right) - \frac{dv_x}{dT} \times \frac{dT}{dx}v_x\tau - v_x\left(T(x)\right) + \frac{dv_x}{dT} \times \frac{dT}{dx}v_x\tau - 2\frac{eE\tau}{m} = 0.
\end{aligned}$$

The electric field one can read,

$$E = -\frac{m}{2e}\frac{dv_x^2}{dT}\frac{dT}{dx} = -\frac{1}{3e}\frac{d\varepsilon}{dT}\frac{dT}{dx}. \tag{2.34}$$

The thermo-power can be written as,

$$S = -\frac{k_B}{2e}, \tag{2.35}$$

i.e., $S = -0.4 \times 10^{-4}$volt/k. We can see that when we apply quantum mechanical models the value of S is 100 times less than this classical Drude's result.

2.3.3 Semi-classical approach

We do need quantum mechanics to understand the properties of metals. We discuss here a quick review of Bloch theory, and then the Boltzmann approach to understand the transport of particles.

2.3.3.1 Bloch Theory

The Bloch theory of electrons concerns the motion of non-interacting electrons in a periodic potential $V(\vec{r})$ generated by ions rather than a free space motion where

the potential is zero. The potential is periodic,

$$V(\vec{r}+\vec{R}) = V(\vec{r}). \tag{2.36}$$

The Hamiltonian of a single electron moving in a periodic potential is,

$$\mathcal{H} = \frac{\vec{p}^2}{2m} + V(\vec{r}). \tag{2.37}$$

According to the Bloch theorem, the translation symmetry of the Hamiltonian allows the wave function of the form,

$$\Psi_{nk}(\vec{r}) = \exp(i\vec{k}\cdot\vec{r})u_{nk}(\vec{r}). \tag{2.38}$$

Where n is band index, and $u_{nk}(\vec{r})$ is a periodic function of period $\vec{R}$. Here $\vec{R}$ is a Bravais lattice vector. The dynamics of the Bloch electrons can be summarised in three phrases. Firstly, the band index is constant of motion. An electron starting its motion in band n will remain thereafter in same band. Second, the position of Bloch electrons changes according to the equation,

$$\vec{v}(\vec{k}) = \frac{1}{\hbar}\frac{\partial\varepsilon}{\partial\vec{k}}, \tag{2.39}$$

and the electron's momentum changes accordingly,

$$\hbar\dot{\vec{k}} = -e\vec{E} - \frac{e}{c}\left(\vec{v}\times\vec{B}\right). \tag{2.40}$$

This is the quantum version of Newton's law. The filling factor of any Bloch state is,

$$f^0(\vec{k}) = \frac{1}{\exp\left(\frac{\varepsilon(\vec{k})-\mu}{k_BT}\right)+1}. \tag{2.41}$$

2.4 Boltzmann Transport

The Boltzmann transport equation tells how particles and energy are transported in any system which obeys the Hamilton's equation. This must not include just the dynamics of carriers under the influence of external fields, but also scattering effects arising from the carrier interactions with impurities, phonons, contacts, etc. The Boltzmann equation is a transport theory that operates in the classical diffusive regime in which the state of a system is described by a non-equilibrium distribution function $f(\mathbf{r},\mathbf{k},t)$, which gives occupancy of a state $\vec{k}$ at position $\vec{r}$

and time t. The position $\vec{r}$ in $f(\mathbf{r}, \mathbf{k}, t)$ represents a suitable coarse grained length scale (much greater than the atomic scale), such that each $\vec{r}$ represents a thermodynamics system.

In equilibrium, $f(\mathbf{r}, \mathbf{k}, t) = f^0(\mathbf{k})$. There are external forces acting to drive the distribution function away from equilibrium and collisions act to restore the equilibrium, i.e., try to bring f back to f^0.

2.4.1 Time evolution of $f(\mathbf{r}, \mathbf{k}, t)$

Suppose we know $f(\mathbf{r}, \mathbf{k}, t)$ at time $t = 0$, we want to know $f(\mathbf{r}, \mathbf{k}, t)$ at some later time t provided we know the forces acting on the system. The electron's position and momentum change continuously and are described by semi-classical equation of motion. The change in distribution function is,

$$df = \frac{\partial f}{\partial t} dt + d\vec{r} \cdot \frac{\partial f}{\partial \vec{r}} + d\vec{k} \cdot \frac{\partial f}{\partial \vec{k}}. \tag{2.42}$$

Thus,

$$\frac{df}{dt} = \frac{\partial f}{\partial t} dt + \dot{\vec{r}} \cdot \frac{\partial f}{\partial \vec{r}} + \dot{\vec{k}} \cdot \frac{\partial f}{\partial \vec{k}}. \tag{2.43}$$

If there are no scattering processes, the total time derivative of distribution function is zero, i.e.,

$$\frac{df}{dt} = 0. \tag{2.44}$$

Hence,

$$\frac{\partial f}{\partial t} = -\dot{\vec{r}} \cdot \frac{\partial f}{\partial \vec{r}} - \dot{\vec{k}} \cdot \frac{\partial f}{\partial \vec{k}}. \tag{2.45}$$

If scattering processes are there, electrons momentum now changes discontinuously, to include the effect of these processes Boltzmann added a new term,

$$\frac{df}{dt}\Big|_{coll} \tag{2.46}$$

called the collision term, the equation (2.45) becomes,

$$\frac{\partial f}{\partial t} = -\dot{\vec{r}} \cdot \frac{\partial f}{\partial \vec{r}} - \dot{\vec{k}} \cdot \frac{\partial f}{\partial \vec{k}} + \frac{df}{dt}\Big|_{coll}. \tag{2.47}$$

The equation (2.47) is known as the Boltzmann equation. We will solve it in the relaxation time approximation where the simplest form of the collision term is,

$$\frac{df}{dt}\,|_{coll} = -\frac{f - f^0}{\tau_\varepsilon}, \tag{2.48}$$

here τ_ε is the relaxation time and depends upon $\vec{k}$ through energy. We will discuss it later. Once the relaxation time approximation is employed, the Boltzmann equation takes a simpler form,

$$\frac{df}{dt} = -\frac{f - f^0}{\tau_\varepsilon}. \tag{2.49}$$

The solution of the above equation in relaxation time approximation can be taken as,

$$f = \int_{-\infty}^{t} dt' f(t') \frac{\exp\left(\frac{t-t'}{\tau_\varepsilon}\right)}{\tau_\varepsilon}. \tag{2.50}$$

Integrating by parts and by using equation (2.45) one can write,

$$f(\vec{r}, \vec{k}, t) = f^0(\vec{k}) - \int_{-\infty}^{t} dt' \exp\left(\frac{t-t'}{\tau_\varepsilon}\right) \left[\dot{\vec{r}} \cdot \frac{\partial}{\partial \vec{r}} + \dot{\vec{k}} \cdot \frac{\partial}{\partial \vec{k}}\right] f^0(t'). \tag{2.51}$$

If we use,

$$\frac{\partial f}{\partial \vec{r}} = \frac{\partial f}{\partial \varepsilon}\left[-\vec{\nabla}\mu - (\varepsilon_{\mathbf{k}} - \mu)\frac{\vec{\nabla}T}{T}\right] \tag{2.52}$$

and

$$\frac{\partial f}{\partial \vec{k}} = \frac{\partial f}{\partial \varepsilon_{\vec{k}}} \hbar \vec{v}, \tag{2.53}$$

thus we obtain,

$$f(\vec{r}, \vec{k}, t) = f^0(\vec{k}) - \int_{-\infty}^{t} dt' \exp\left(\frac{t-t'}{\tau_\varepsilon}\right) \left[\vec{r} \cdot \left(-\vec{\nabla}\mu - (\varepsilon - \mu)\frac{\vec{\nabla}T}{T}\right)\frac{\partial f}{\partial \varepsilon} + \hbar\dot{\vec{k}} \cdot \vec{v}\frac{\partial f}{\partial \varepsilon}\right]. \tag{2.54}$$

By using equation (2.40) we obtain,

$$\hbar\dot{\vec{k}} \cdot \vec{v} = -e\vec{v} \cdot \vec{E}. \tag{2.55}$$

Hence,

$$f = f^0 - \int_{-\infty}^{t} dt' \exp\left(\frac{t-t'}{\tau_\varepsilon}\right) \vec{v}_{\mathbf{k}} \cdot \left[e\left(\vec{E} + \frac{\vec{\nabla}\mu}{e}\right) + \frac{\varepsilon_{\vec{k}} - \mu}{T}\vec{\nabla}T\right]\left(-\frac{\partial f}{\partial \varepsilon}\right). \tag{2.56}$$

We take the slow variation of semi-classical dynamics such that we ignore the time dependence of all other quantities except exponential factor. By integrating above equation, only exponential factor, we have

$$f = f^0 + \tau_\varepsilon \mathbf{v_k} \cdot \left[e\vec{E'} + \frac{\varepsilon - \mu}{T} \vec{\nabla} T \right] \left(\frac{\partial f}{\partial \varepsilon} \right). \tag{2.57}$$

We define here,

$$\vec{E'} = \vec{E} + \frac{\vec{\nabla} T}{e}. \tag{2.58}$$

This form of solution has the virtue that it is written as a sum of unperturbed term and perturbed term. Now, let's formulate how we can calculate τ_ε. Consider V_I is the impurity potential which causes the transition from one Bloch state to another. The rate of transition from $\vec{k} \to \vec{k'}$ is,

$$W_{\vec{k} \to \vec{k'}} = \frac{2\pi}{\hbar} \mid \langle \mathbf{k'} | V_I | \mathbf{k} \rangle \mid^2 \delta \left(\varepsilon(\vec{k}) - \varepsilon(\vec{k'}) \right). \tag{2.59}$$

This is Fermi's golden rule. Now let's look back on the collision term, we can write it more elaborately as,

$$\frac{df}{dt} \mid_{coll} = \frac{1}{(2\pi)^3} \int d^3\vec{k'} W_{\vec{k} \to \vec{k'}} \left(f(\vec{k}) - f(\vec{k'}) \right). \tag{2.60}$$

As the temperature does not affect much the impurity scattering so we can ignore the temperature dependent term in (2.57) to get,

$$\frac{df}{dt} \mid_{coll} = -\frac{e}{\hbar} \frac{\partial f}{\partial \varepsilon} \mathbf{v(k)} \cdot \mathbf{E}_{eff} \tag{2.61}$$

and,

$$f(\mathbf{k}) - f(\mathbf{k'}) = -\frac{\tau_\varepsilon e}{\hbar} \frac{\partial f^0}{\partial \varepsilon} \left[v(\mathbf{k}) - v(\mathbf{k'}) \right] \cdot \mathbf{E}_{eff}. \tag{2.62}$$

Using (2.61) and (2.62) one can solve (2.60) for τ_ε,

$$\frac{1}{\tau_\varepsilon} = \frac{1}{(2\pi)^3} \int d^3\vec{k'} W_{\vec{k} \to \vec{k'}} \left(1 - \cos\theta \right). \tag{2.63}$$

Here, θ is angle between $\vec{k}$ and $\vec{k'}$.

2.4.2 Thermodynamics and production of heat

As pioneered by Massieu and Gibbs, thermodynamics can be based on the postulate that the static properties of any physical system with r independent variables can be compressed into certain functions of these variables, which are called thermodynamic potentials. The most familiar thermodynamic potential is the energy ε when expressed as a function of the independent extensive variables of the system. In the case of simple fluid or gas, the independent extensive variables are the entropy S, the volume V and the particle number N. Assigning values for a set of independent variables, e.g., for (S, V, N), specifies a certain state of the system. The total differential of the function $\varepsilon(S, V, N)$ can be written as,

$$d\varepsilon = \frac{\partial \varepsilon}{\partial S} dS + \frac{\partial \varepsilon}{\partial V} dV + \frac{\partial \varepsilon}{\partial N} dN. \tag{2.64}$$

For a fixed volume this equation reduces as,

$$d\varepsilon = \frac{\partial \varepsilon}{\partial S} dS + \frac{\partial \varepsilon}{\partial N} dN. \tag{2.65}$$

If we define the absolute temperature as

$$T(S, N) = \frac{\partial \varepsilon}{\partial S}, \tag{2.66}$$

and the chemical potential μ as

$$\mu(S, N) = \frac{\partial \varepsilon}{\partial N}, \tag{2.67}$$

then the equation (2.65) becomes,

$$d\varepsilon = TdS + \mu dN. \tag{2.68}$$

Equation (2.66) and (2.67) are called caloric and chemical equations of state of the system. The equation (2.68) is called the Gibbs fundamental form. This equation has a very simple physical meaning. Consider a system heated by connecting it to an external reservoir by keeping volume V and number of particles N fixed. Suppose that an amount $\Delta\varepsilon = T\Delta S$, of energy, along with an amount of ΔS of entropy, has to be added to the system from the reservoir. The first law of thermodynamics can be written in the form

$$T\frac{\partial S}{\partial t} = \frac{\partial \varepsilon}{\partial t} - \mu \frac{\partial N}{\partial t}. \tag{2.69}$$

Now we discuss conservation laws. In general any balanceable X has to obey continuity equation of the form

$$\frac{\partial X(t,\vec{r})}{\partial t} + \nabla \cdot \vec{j}_X(t,\vec{r}) = \dot{X}, \tag{2.70}$$

where $\vec{j}_X(t,\vec{r})$ is the local X-current density and $\dot{X}$ is the X generation rate. For conserved quantities $\dot{X}$ vanishes. The continuity equation for the ε is

$$\frac{\partial \varepsilon}{\partial t} + \nabla \cdot \vec{j}_\varepsilon = \dot{\varepsilon}, \tag{2.71}$$

for the number of particles

$$\frac{\partial N}{\partial t} + \nabla \cdot \vec{j}_N = \dot{N}, \tag{2.72}$$

and for the entropy is

$$\frac{\partial S}{\partial t} + \nabla \cdot \vec{j}_S = \dot{S}. \tag{2.73}$$

Define,

$$\vec{j}_N = N\vec{v}, \tag{2.74}$$

and

$$\vec{j}_\varepsilon = \varepsilon\vec{v}. \tag{2.75}$$

We assume here energy is transported with the same velocity as the particle current. Since the number of particles are fixed, so N is a conserved quantity, i.e., $\dot{N}$ is zero. Let $\vec{F}$ be the external force acting on the system which is usually electric or magnetic force. Then the rate of the energy generation can be written as

$$\dot{\varepsilon} = N\vec{F} \cdot \vec{v} = \vec{F} \cdot \vec{j}_N. \tag{2.76}$$

The equations of continuity for energy and particle currents becomes,

$$\frac{\partial N}{\partial t} + \nabla \cdot \vec{j}_N = 0, \tag{2.77}$$

$$\frac{\partial \varepsilon}{\partial t} + \nabla \cdot \vec{j}_\varepsilon = \vec{F} \cdot \vec{j}_N. \tag{2.78}$$

By combining the equations (2.69), (2.77) and (2.78) we have,

$$T\frac{\partial S}{\partial t} - \mu\vec{\nabla} \cdot \vec{j}_N + \vec{\nabla} \cdot \vec{j}_\varepsilon = \vec{F} \cdot \vec{j}_N. \tag{2.79}$$

If we define the entropy current as

$$\vec{j}_S = \frac{\vec{j}_\varepsilon - \mu \vec{j}_N}{T}. \tag{2.80}$$

This easily follows from equation (2.68) and multiplying by $\vec{v}$. Then, the continuity equation for the entropy becomes

$$\dot{S} = \frac{\partial S}{\partial t} + \vec{\nabla} \cdot \left(\frac{\vec{j}_\varepsilon - \mu \vec{j}_N}{T} \right), \tag{2.81}$$

$$= \frac{\partial S}{\partial t} + \left(\frac{1}{T}\right) \vec{\nabla} \cdot \vec{j}_\varepsilon + \vec{j}_\varepsilon \cdot \vec{\nabla} \left(\frac{1}{T}\right) - \vec{\nabla} \left(\frac{\mu}{T}\right) \cdot \vec{j}_N - \left(\frac{\mu}{T}\right) \vec{\nabla} \cdot \vec{j}_N. \tag{2.82}$$

By using equation (2.79), the above equation simplifies to give,

$$\dot{S} = \frac{\vec{F} \cdot \vec{j}_N}{T} + \vec{j}_\varepsilon \cdot \vec{\nabla} \left(\frac{1}{T}\right) - \vec{\nabla} \left(\frac{\mu}{T}\right) \cdot \vec{j}_N. \tag{2.83}$$

If $\vec{F}$ is identified as electromagnetic force

$$\vec{F} = -e \left(\vec{E} + \frac{\vec{v} \times \vec{B}}{c} \right), \tag{2.84}$$

then,

$$\vec{F} \cdot \vec{j}_N = -\frac{e}{T} \vec{E} \cdot \vec{j}_N. \tag{2.85}$$

The rate at which entropy is generated can be written as:

$$\dot{S} = \frac{1}{T} \left(e\vec{E} + \vec{\nabla}\mu + \frac{\vec{\nabla}T}{T} \left(\frac{\varepsilon}{N} - \mu \right) \right) \cdot \vec{j}_N. \tag{2.86}$$

And the heat generated $\dot{Q}$ per time is,

$$\dot{Q} = T\frac{\dot{S}}{V} = -\left[e\vec{E} + \vec{\nabla}\mu + \frac{\vec{\nabla}T}{T} \left(\frac{\varepsilon}{N} - \mu \right) \right] \cdot \frac{\vec{j}_N}{V}. \tag{2.87}$$

Define,

$$\dot{Q}(\vec{k}) = -\left[e\vec{E} + \vec{\nabla}\mu + \frac{\vec{\nabla}T}{T} \left(\varepsilon_{\vec{k}} - \mu \right) \right] \cdot \frac{\vec{j}_N}{V} \tag{2.88}$$

to be heat production per wavenumber per volume. Here $\varepsilon_{\vec{k}}$ is energy per particle with wavenumber $\vec{k}$.

2.5 Thermoelectric phenomenon

Consider a solid immersed in forcing fields, such as an electric or magnetic or a thermal gradient. We want to check what response should be associated with each of the forcing field. For example, applying thermal gradient will in general produce an electric current as well. To calculate these effects, one should check the flux associated with each of the forcing field. We define, the flux induced by a forcing field to be the derivative of heat. In general, let Y_β be the flux associated with the forcing field y_β, then the flux Y_β is defined as:

$$Y_\beta = \frac{d\dot{Q}(\vec{k})}{dy_\beta} \tag{2.89}$$

There are three forcing fields considered in equation(2.86), $\vec{E}, \vec{\nabla}$ and $\vec{\nabla}\mu$. Since $\vec{E}$ and $\vec{\nabla}\mu$ appear in the combination $\vec{E} + \vec{\nabla}\mu$, so it is useful to define the electrochemical force

$$\vec{E}' = \vec{E} + \frac{\vec{\nabla}\mu}{e}. \tag{2.90}$$

Now it is straightforward to calculate the flux associated with the electrochemical force. By using equation (2.89) and (2.88) we have,

$$\begin{aligned} \vec{j}_e &= -e\frac{\vec{j}_N}{V}, \\ &= -\frac{2e}{(2\pi)^3}\int d^3\vec{k}\vec{v}(\vec{k})f(\vec{k}). \end{aligned} \tag{2.91}$$

Here, 2 is a factor due to spin. By writing $f(\vec{k})$ as

$$f(\vec{k}) = f^0(\vec{k}) + f^1(\vec{k}), \tag{2.92}$$

i.e., the sum of perturbed and unperturbed part, we have,

$$\vec{j}_e = -\frac{2e}{(2\pi)^3}\int d^3\vec{k}\vec{v}(\vec{k})\left(f^0(\vec{k}) + f^1(\vec{k})\right). \tag{2.93}$$

Since equilibrium part of the distribution function generates no current, the first part of the integral in equation (2.93) vanishes, then

$$\vec{j}_e = -\frac{2e}{(2\pi)^3}\int d^3\vec{k}\vec{v}(\vec{k})f^1(\vec{k}) = \frac{2e}{(2\pi)^3}\int d^3\vec{k}\vec{v}(\vec{k})\left(f(\vec{k}) - f^0(\vec{k})\right). \tag{2.94}$$

With the help of equation (2.57), we can write the above equation as:

$$\vec{j}_e = \frac{2e}{(2\pi)^3}\int d^3\vec{k}\vec{v}(\vec{k})\tau_\varepsilon\vec{v}(\vec{k})\cdot\left[e\vec{E}' + \frac{\varepsilon_{\vec{k}}-\mu}{T}\left(-\vec{\nabla}T\right)\right]\left(\frac{\partial f}{\partial\mu}\right). \tag{2.95}$$

We use here the fact that

$$-\frac{\partial f}{\partial\varepsilon_{\vec{k}}} = \frac{\partial f}{\partial\mu}. \tag{2.96}$$

Now it is conventional to take $-\frac{\vec{\nabla}T}{T}$ as force. The flux associated with this force is

$$\vec{j}_Q = \frac{\vec{j}_\varepsilon - \mu\vec{j}_N}{V} = \frac{2}{(2\pi)^3}\int d^3\vec{k}\vec{v}(\vec{k})(\varepsilon_{\vec{k}}-\mu)f(\vec{k}). \tag{2.97}$$

This equation can easily be simplified in a similar way as we did before for the electric current. The simplified form of the above equation is:

$$\vec{j}_Q = \frac{2}{(2\pi)^3}\int d^3\vec{k}\vec{v}(\vec{k})(\varepsilon_{\vec{k}}-\mu)\tau_\varepsilon\vec{v}(\vec{k})\cdot\left[-e\vec{E}' + \frac{\varepsilon_{\vec{k}}-\mu}{T}\left(-\vec{\nabla}T\right)\right]\left(\frac{\partial f}{\partial\mu}\right). \tag{2.98}$$

Equation (2.95) and (2.98) can be written as:

$$\vec{j}_e = \frac{2e}{(2\pi)^3}\int d^3\vec{k}\vec{v}_{\vec{k}}\tau_\varepsilon\vec{v}_{\vec{k}}\cdot\left[e\vec{E}' + \frac{\varepsilon_{\vec{k}}-\mu}{T}\left(-\vec{\nabla}T\right)\right]\left(\frac{\partial f}{\partial\mu}\right), \tag{2.99}$$

$$\vec{j}_Q = \frac{2}{(2\pi)^3}\int d^3\vec{k}\vec{v}_{\vec{k}}\vec{v}_{\vec{k}}\tau_\varepsilon\vec{v}_{\vec{k}}\cdot\left[-e(\varepsilon_{\vec{k}}-\mu)\vec{E}' + \frac{(\varepsilon_{\vec{k}}-\mu)^2}{T}\left(-\vec{\nabla}T\right)\right]\left(\frac{\partial f}{\partial\mu}\right). \tag{2.100}$$

If we define a new integral,

$$\mathfrak{L}^{(\nu)}_{\alpha\beta} = \frac{2e^2}{(2\pi)^3}\int\int d^3\vec{k}v_\alpha v_\beta\tau_\varepsilon\left(\varepsilon_{\vec{k}}-\mu\right)^\nu\left(\frac{\partial f}{\partial\mu}\right), \tag{2.101}$$

then the equations(2.99) and (2.100) becomes,

$$\begin{aligned} j_{e\alpha} &= \mathfrak{L}^{(0)}_{\alpha\beta}E'_\beta - \frac{1}{e}\mathfrak{L}^{(1)}_{\alpha\beta}\left(-\frac{(\nabla T)_\beta}{T}\right), \\ j_{Q\alpha} &= -\frac{1}{e}\mathfrak{L}^{(1)}_{\alpha\beta}E'_\beta + \frac{1}{e^2}\mathfrak{L}^{(2)}_{\alpha\beta}\left(-\frac{(\nabla T)_\beta}{T}\right). \end{aligned} \tag{2.102}$$

The matrix form of the above equation is,

$$\begin{pmatrix} \vec{j}_e \\ \vec{j}_Q \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}\begin{pmatrix} \vec{E}' \\ \frac{\vec{\nabla}T}{T} \end{pmatrix}. \tag{2.103}$$

Where

$$A_{11} = \mathfrak{L}^{(0)}, \quad A_{12} = A_{21} = -\frac{1}{e}\mathfrak{L}^{(1)}, \quad A_{22} = \frac{1}{e^2}\mathfrak{L}^{(2)}. \tag{2.104}$$

Defining

$$\sigma_{\alpha\beta}(\varepsilon) = \frac{2e}{(2\pi)^3}\int d^3\vec{k} v_\alpha v_\beta \tau_\varepsilon \delta(\varepsilon - \varepsilon_{\vec{k}}), \tag{2.105}$$

we have

$$\mathfrak{L}^{\nu}_{\alpha\beta} = \int d\varepsilon \frac{\partial f}{\partial \mu}(\varepsilon - \mu)^\nu \sigma_{\alpha\beta}(\varepsilon). \tag{2.106}$$

The above integral is evaluated for different values of ν here. For $\nu = 0$,

$$\mathfrak{L}^{0}_{\alpha\beta} = \int d\varepsilon \frac{\partial f}{\partial \mu}\sigma_{\alpha\beta}(\varepsilon). \tag{2.107}$$

If we use the fact that at temperature well below Fermi temperature

$$\frac{\partial f}{\partial \mu} = \delta(\varepsilon - \varepsilon_F), \tag{2.108}$$

where ε_F is Fermi energy, we obtain,

$$\mathfrak{L}^{0}_{\alpha\beta} = \int d\varepsilon \delta(\varepsilon - \varepsilon_F)\sigma_{\alpha\beta}(\varepsilon). \tag{2.109}$$

Hence,

$$\mathfrak{L}^{(0)}_{\alpha\beta} = \sigma_{\alpha\beta}(\varepsilon_F). \tag{2.110}$$

For $\nu = 1$, the integral in equation (2.106) is,

$$\mathfrak{L}^{(1)}_{\alpha\beta} = \int d\varepsilon \frac{\partial f}{\partial \mu}(\varepsilon - \mu)\sigma_{\alpha\beta}(\varepsilon). \tag{2.111}$$

This integral vanishes if we ignore the energy dependence of, $\sigma_{\alpha\beta}(\varepsilon)$. To make it meaningful we expand $\sigma_{\alpha\beta}(\varepsilon)$ around Fermi energy, i.e.,

$$\sigma_{\alpha\beta}(\varepsilon) = \sigma_{\alpha\beta}(\varepsilon = \varepsilon_F) + (\varepsilon - \mu)\frac{d\sigma_{\alpha\beta}(\varepsilon = \varepsilon_F)}{d\varepsilon}. \tag{2.112}$$

Hence,

$$\mathfrak{L}^{(1)}_{\alpha\beta} = \int d\varepsilon \frac{\partial f}{\partial \mu}(\varepsilon - \mu)\left(\sigma_{\alpha\beta}(\varepsilon = \varepsilon_F) + (\varepsilon - \mu)\frac{d\sigma_{\alpha\beta}(\varepsilon = \varepsilon_F)}{d\varepsilon}\right). \tag{2.113}$$

The first term in this integral vanishes by integrating because it contains an odd power of $(\varepsilon - \mu)$. Thus,

$$\mathfrak{L}^{(1)}_{\alpha\beta} = \int d\varepsilon \frac{\partial f}{\partial \mu}(\varepsilon - \mu)^2 \frac{d\sigma_{\alpha\beta}(\varepsilon = \varepsilon_F)}{d\varepsilon}. \tag{2.114}$$

Since,

$$\frac{\partial f}{\partial \mu} = \frac{1}{k_B T} \frac{\exp\left(\frac{\varepsilon-\mu}{k_B T}\right)}{\left(\exp\left(\frac{\varepsilon-\mu}{k_B T}\right)+1\right)^2}, \tag{2.115}$$

thus,

$$\mathfrak{L}^{(1)}_{\alpha\beta} = \int d\varepsilon \frac{1}{k_B T} \frac{\exp\left(\frac{\varepsilon-\mu}{k_B T}\right)}{\left(\exp\left(\frac{\varepsilon-\mu}{k_B T}\right)+1\right)^2}(\varepsilon - \mu)^2 \frac{d\sigma_{\alpha\beta}(\varepsilon = \varepsilon_F)}{d\varepsilon}. \tag{2.116}$$

If we define $x = \frac{\varepsilon-\mu}{k_B T}$, then, the above equation becomes,

$$\mathfrak{L}^{(1)}_{\alpha\beta} = \int dx \frac{x^2 \exp x}{(\exp x + 1)^2} \frac{d\sigma_{\alpha\beta}(\varepsilon = \varepsilon_F)}{d\varepsilon}. \tag{2.117}$$

Hence,

$$\mathfrak{L}^{(1)}_{\alpha\beta} = \frac{\pi^2}{3}(k_B T)^2 \frac{d\sigma_{\alpha\beta}}{d\varepsilon} \mid_{\varepsilon=\varepsilon_F}. \tag{2.118}$$

For $\nu = 2$, equation (2.106) is,

$$\mathfrak{L}^{(2)}_{\alpha\beta} = \int d\varepsilon \frac{\partial f}{\partial \mu}(\varepsilon - \mu)^2 \sigma_{\alpha\beta}(\varepsilon). \tag{2.119}$$

Again by using the expansion of $\sigma_{\alpha\beta}(\varepsilon)$, the above integral can be written as:

$$\mathfrak{L}^{(2)}_{\alpha\beta} = \int d\varepsilon \frac{\partial f}{\partial \mu}(\varepsilon - \mu)^2 \left(\sigma_{\alpha\beta}(\varepsilon = \varepsilon_F) + (\varepsilon - \mu)\frac{d\sigma_{\alpha\beta}(\varepsilon = \varepsilon_F)}{d\varepsilon}\right). \tag{2.120}$$

The second term in this integral vanishes because it contains an odd power of $(\varepsilon - \mu)$. Hence,

$$\mathfrak{L}^{(2)}_{\alpha\beta} = \int d\varepsilon \frac{\partial f}{\partial \mu}(\varepsilon - \mu)^2 \sigma_{\alpha\beta}(\varepsilon = \varepsilon_F). \tag{2.121}$$

This integral is already solved above. Thus,

$$\mathfrak{L}^{(2)}_{\alpha\beta} = \frac{\pi^2}{3}(k_B T)^2 \sigma_{\alpha\beta}(\varepsilon_F). \tag{2.122}$$

First, consider a situation where $\vec{\nabla}T = 0$ in (2.103), we obtain

$$\vec{j}_e = A_{11}\vec{E}'. \tag{2.123}$$

One can reads the electrical conductivity from the above equation

$$\sigma = A_{11} \tag{2.124}$$

Now, notice that a pure electrochemical gradient causes heat flow, and a pure thermal gradient causes current to flow. We discussed earlier that thermal conductivity is measured in open circuit configuration. Therefore, to get required thermal conductivity coefficient, we put $j_e = 0$ in Eq. (2.103)

$$0 = A_{11}\vec{E}' + A_{12}\left(\frac{-\vec{\nabla}T}{T}\right), \tag{2.125}$$

This implies that

$$\vec{E}' = (A_{11})^{-1}A_{12}\frac{\vec{\nabla}T}{T} \tag{2.126}$$

This shows that a weak field is necessary to oppose the current. In a finite sample, it would automatically result from charge build up at the boundaries. By combining equation (2.103) and (2.126), we obtain

$$\vec{j}_Q = \left(A_{21}(A_{11})^{-1}A_{12} - A_{22}\right)\left(\frac{\vec{\nabla}T}{T}\right) \tag{2.127}$$

By using Fourier's Law one can read the thermal conductivity

$$\kappa = \frac{A_{22} - A_{21}(A_{11})^{-1}A_{12}}{T}, \tag{2.128}$$

the second term in this expression is much smaller than compare to A_{22}, so we neglect this term and by using the equation (2.104) and (2.122), we have

$$\kappa_{\alpha\beta} = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 T\sigma_{\alpha\beta}(\varepsilon = \varepsilon_F) \tag{2.129}$$

This is nothing but well-known Wiedmann-Franz law. We recover Wiedmann-Franz law for Bloch electrons. We can see that Lorenz number $L_0 = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2$ differs by a factor of $\pi^2/3$ from the Drude's result. This simple relation between thermal and electrical conductivity applies component by component to electrical and thermal conductivity so long as the relaxation time approximation is valid.

Up to now, we developed the coefficient of electrical and thermal conductivity, two other co-efficient remain to be investigated thermo-power and Peltier coefficient. Let us suppose that we apply a thermal gradient across a sample, which is in open circuit configuration; i.e., there is no electrical current flow through the circuit. The thermal gradient establishes an electric field **E**:

$$\vec{E}' = (A_{11})^{-1} A_{12} \frac{\vec{\nabla} T}{T} \tag{2.130}$$

By using equation (2.29), one can read the thermo-power or Seebeck coefficient

$$\mathcal{S} = A_{11}^{-1} \frac{A_{12}}{T}. \tag{2.131}$$

By using equation (2.104),(1.118) and (1.22), we can write the above expression of thermo-power as:

$$\mathcal{S}_{\alpha\beta} = -\frac{\pi^2}{3} \frac{k_B^2 T}{e} \frac{1}{\sigma_{\alpha\beta}} \frac{d\sigma_{\alpha\beta}}{d\varepsilon} = -\frac{\pi^2}{3} \frac{k_B^2 T}{e} \left[\frac{d}{d\varepsilon} \ln(\sigma_{\alpha\beta}) \right]_{\varepsilon=\varepsilon_F} \tag{2.132}$$

The measured values of thermo-power are the order of $\mu V K^{-1}$. The Peltier effect arise when current flows in a circuit without temperature gradient. The flow of electrical current induces heat current. The Peltier coefficient is defined by the equation:

$$j_Q = \Pi j_e \tag{2.133}$$

One sees from the equation (2.104) and (2.118)

$$\Pi = A_{21}(A_{11})^{-1} = \frac{\pi^2}{3} \frac{k_B^2 T^2}{e} \left[\frac{\partial}{\partial \varepsilon} (\ln \sigma(\varepsilon)) \right]_{\varepsilon=\varepsilon_F}. \tag{2.134}$$

For the completeness, we state here that Peltier coefficient and Seebeck coefficient related by the equation,

$$\Pi = TS. \tag{2.135}$$

2.6 Mesoscopic Quantum Transport

Any mesoscopic system has its size between microscopic and macroscopic system. The major property of mesoscopic system is that electron's wave function remains phase-coherent all over the sample. This introduces restrictions on the dimension of the system and temperature. For electrons there are two type of description.

First is local current density and electric field. Second is global transport where G conductance relates the total current to voltage. For large homogeneous conductors G and σ are related by the equation:

$$G = \sigma L^{d-2}. \tag{2.136}$$

It is clear that from the equation in two dimension G and σ have the same meaning. For mesoscopic systems, local quantities are meaningless and we discuss only conductance. Here we define three transport regime for electrons.
The first is the ballistic transport regime, where the dimensions of the system are less than the elastic mean free path. The second is the quasi-ballistic regime, where the width of the system is less than the elastic mean free path and the length of the system is greater than the elastic mean free path. The third is the diffusive regime, where the dimensions of the system are greater than the elastic mean free path. We restrict ourself to the ballistic transport regime in our further discussion. The Landauer formula plays an important role in this transport regime. We will explain here Landauer transport, which will be completed in two steps. First we will discuss a simpler model of confinement of electron. Then, secondly we will describe our core business, quantum transport.

2.6.1 Ideal wave guide

Consider an electron confined in a two dimensional rectangular wave guide, which is infinitely long in x-direction. The walls of the wave-guide are impenetrable at $y = \pm\frac{a}{2}$. We can make this by assuming there is an infinite potential,

$$U(y) = \begin{cases} 0 & \frac{-a}{2} < y < \frac{a}{2} \\ \infty & \text{otherwise.} \end{cases} \tag{2.137}$$

The time independent Schrodinger's equation for this system is,

$$\left[\frac{\vec{P}^2}{2m} + U(x)\right]\Psi(x,y) = E\Psi(x,y). \tag{2.138}$$

Since the potential is only x-dependent, we can apply the separation of variables. If we write $\Psi(x,y) = \psi(x)\phi(y)$, this separates into two one dimensional uncoupled

equations,

$$\left[\frac{P_y^2}{2m} + U(y)\right]\phi(y) = \varepsilon_x \phi(y), \tag{2.139}$$

$$\frac{P_x^2}{2m}\psi(x) = \varepsilon_x \psi(x). \tag{2.140}$$

Where ε_x is energy of longitudinal motion and ε_y is energy of transverse motion. The solution of the equation (2.140) are plane waves and can be written as,

$$\psi(x) = \exp(ik_x x), \tag{2.141}$$

and the energy associated with this motion is,

$$\varepsilon_x = \frac{\hbar^2 k_x^2}{2m}. \tag{2.142}$$

The solution of the equation (2.139) is,

$$\phi(y) = \frac{2}{\sqrt{a}} \sin k_y (y - \frac{a}{2}), \tag{2.143}$$

the effect of the infinite potential can be taken into account by setting $\phi(\pm\frac{a}{2}) = 0$. This condition quantize the k_y, i.e.,

$$k_y^n = \frac{n\pi}{a}. \tag{2.144}$$

This shows that longitudinal motion of electron is quantized with the energy eigenvalues labelled by n are

$$\varepsilon_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}. \tag{2.145}$$

Here n is an integer, called number of modes in wavetheory and called channel in mesoscopic physics. Thus, the total energy is the energy of the longitudinal motion shifted by a channel dependent transverse energy given by the equation,

$$E_n(k_y) = \frac{\hbar^2 k_x^2}{2m} + \frac{\hbar^2 \pi^2 n^2}{2ma^2}. \tag{2.146}$$

The complete wave-function can be written as

$$\psi(x, y) = A \exp(ik_x x) \sin k_y^n (y - \frac{a}{2}), \tag{2.147}$$

where A is normalization constant.

2.6.1.1 Quantum point contact

Quantum point contact is a system without potential barrier that behaves as a system with potential barrier. Now we consider a wave guide with variable walls. We assume that as, $x \to \pm\infty$ the width of the wave guide has a constant value a_0 as one moves towards moves towards $x = 0$, these walls come closer and form a constriction, as shown in fig. (2.1). The potential for this system can be written

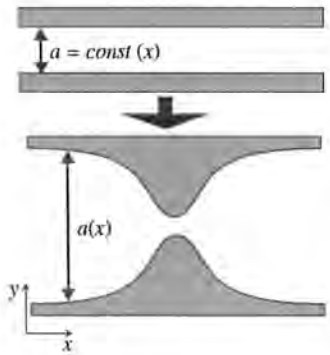

FIGURE 2.1: From a waveguide to constant dimension to adiabatic waveguide.

as,

$$U(y) = \begin{cases} 0 & \frac{-a(x)}{2} < x < \frac{a(x)}{2} \\ \infty & otherwise. \end{cases} \tag{2.148}$$

Now the wave function of Schrodinger equation (2.138) is not separable, so previous argument is not valid. However, we can understand generally the quantum point contact by considering an adiabatic wave guide[24], i.e. the length scale at which the dimension varies is much less than the dimension themselves:

$$|a(x)'|<<1, \qquad a(x)|a(x)''|<<1. \tag{2.149}$$

If these approximations hold then the walls are locally flat and parallel. The wave functions are separable and we can approximate the solutions with the solutions for an ideal wave guide. The wave function can be written as

$$\Psi(x,y) = \psi(x)\phi\left(y, a(x)\right), \tag{2.150}$$

where the transverse wave-function is given by equation (2.143) by replacing $a \to a(x)$, i.e.,

$$\phi_n(y, a(x)) = \frac{2}{\sqrt{a(x)}} \sin k_y^n \left(y - a(x)\right). \tag{2.151}$$

The local energy eigenvalues corresponds to this wave-function are,

$$\varepsilon_n(x) = \frac{\hbar^2 \pi^2 n^2}{2ma(x)^2}. \tag{2.152}$$

This energy depends upon the channel index and x through the dimension of the wave guide. The longitudinal wave-function $\psi(x)$ satisfy the equation

$$\left[\frac{P_x^2}{2m} + \varepsilon_n(x)\right] \psi(x) = E\psi(x). \tag{2.153}$$

We can see that $\varepsilon_n(x)$ plays the role of potential energy which depends upon channel index. Note that for every value of n this potential energy forms a barrier near the constriction at $x = 0$, as shown in fig(2.2).

The above equation can be written as,

$$\left[\frac{P_y^2}{2m} - (E - \varepsilon_n)\right] \psi(y) = 0, \tag{2.154}$$

$$\left[\frac{d^2}{dy^2} + \frac{2m}{\hbar^2} (E - \varepsilon_n)\right] \psi(y) = 0. \tag{2.155}$$

If we define,

$$k^2 = \frac{2m}{\hbar^2} ((E - \varepsilon_n)). \tag{2.156}$$

The above equation becomes,

$$\left[\frac{d^2}{dx^2} + k^2\right] \psi(x) = 0. \tag{2.157}$$

Let us consider a situation for which a given energy E is greater than the maximum barrier height for some value of n. The solution of the above equation is,

$$\psi(x) = \begin{cases} A\exp(ikx) + B\exp(-ikx), & x<0 \\ C\exp(ikx), & x > 0. \end{cases} \tag{2.158}$$

To calculate the values of A, B and C , we use the boundary conditions,

$$\psi_1(0) = \psi_2(0), \qquad \frac{d\psi_1(0)}{dx} = \frac{d\psi_2(0)}{dx}, \tag{2.159}$$

equation(2.140) gives,

$$A + B = C, \qquad A - B = 0, \tag{2.160}$$

hence, $B = 0$ and $C = A$. If we define transmission and reflection coefficient in a usual way, we have $T = 1$ and $R = 0$. Thus, an incident electron with energy

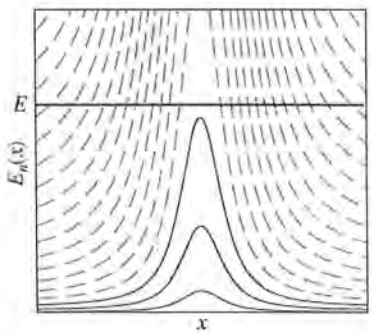

FIGURE 2.2: Channel dependent potential energy.

greater than the maximal barrier height will completely pass through it. On the other way, if we assume impenetrable barrier, an incoming electron with energy less than the maximal of the barrier height, will reflected back. Therefore, an adiabatic wave-guide appears to be same as an ideal wave-guide with a potential barrier. Generally, for each channel we define a transmission coefficient $T_n(E)$ which depends upon channel index. Here in this case $T_n(E) = 1$ for open channel and, $T_n(E) = 0$ for a closed channel. Significantly, the electrons are perfectly reflected in a closed channel even in the absence of a potential barrier.

2.7 Quantum transport

Here we are going to study our main business the quantum transport. As we know that the current density is,

$$\begin{aligned} j_x =& 2e \int \frac{d^2\mathbf{k}}{(2\pi)^2} v_x(k_y) f_n(k_x), \\ =& 2e \int \frac{dk_x}{2\pi} \frac{dk_y}{2\pi} v_x(k_x) f_n(k_x). \end{aligned} \tag{2.161}$$

Here 2 is a factor due to spin, $f_n(k_x)$ is filling factor and $v_x(k_x)$ is speed of the electrons in the x-direction. The expression for the velocity in the x-direction can

be found by using Heisenberg EOM,

$$\begin{aligned} i\hbar\dot{x} &= [x, H(p_x, p_y, x, y)], \\ &= [x, p_x]\frac{\partial H}{\partial p_x} + [x, p_y]\frac{\partial H}{\partial p_y} + [x, x]\frac{\partial H}{\partial x} + [x, y]\frac{\partial H}{\partial y}, \\ &= i\hbar\frac{\partial H}{\partial p_x}, \\ \dot{x} &= \frac{\partial H}{\partial p_x}. \end{aligned} \tag{2.162}$$

Hence,

$$v_x = \frac{1}{\hbar}\frac{\partial E}{\partial k_x}. \tag{2.163}$$

Note that we can use any cross-section to evaluate the current because charge conservation states that current through any cross-section remains same. We choose the cross-section far above from the constriction where $a(x)$ has a constant value a_0, so does k_y. Hence,

$$\int_{-\infty}^{+\infty}\frac{dk_y}{2\pi} \to \frac{1}{a_0}\sum_n. \tag{2.164}$$

Thus, the expression for the current density becomes,

$$j_x = \frac{2e}{a}\sum_n\int_{-\infty}^{+\infty}\frac{dk_x}{2\pi}v(k_x)f_n(k_x). \tag{2.165}$$

One can read the expression for the current as,

$$I_x = 2e\sum_n\int_{-\infty}^{+\infty}\frac{dk_x}{2\pi}v(k_x)f_n(k_x). \tag{2.166}$$

Since closed channels do not contribute to the flow of current, we focus only on open channels. Let us connect the wave-guide with two reservoirs which are at chemical potentials μ_L and μ_R. Where, μ_L is the chemical potential of the left reservoir and μ_R is the chemical potential of the lower reservoir as shown in fig(2.3). These reservoirs injected electrons into the wave-guide.

Now the filling factor of the electrons which are injected by the left reservoir

$$f_L(E) = f_n(E - \mu_A), \tag{2.167}$$

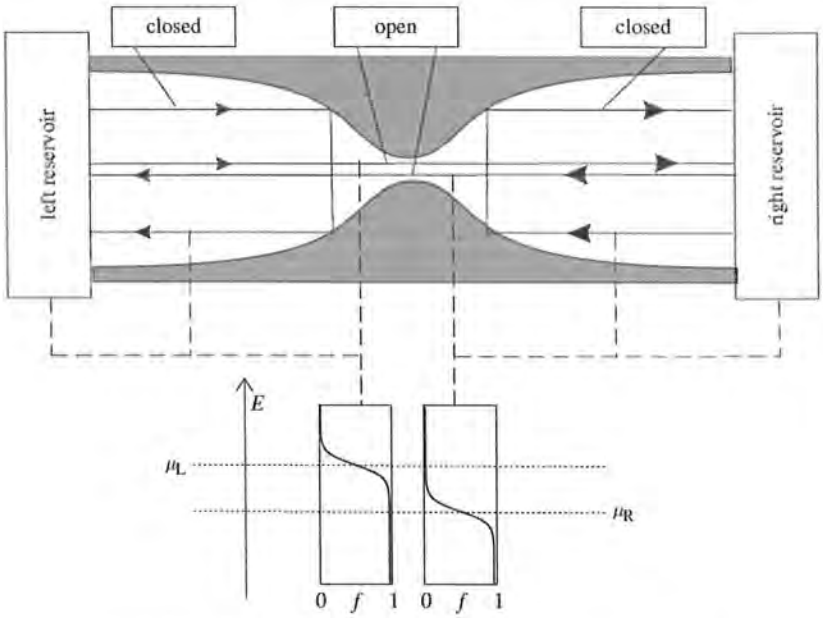

FIGURE 2.3: filling factors for open and close channels.

and the filling factor of the electrons which are injected by the right reservoir

$$f_R(E) = f_n(E - \mu_B). \tag{2.168}$$

Since filling factor depends upon energy and energy is labelled by n so there is n dependence in the filling factor. Let I_+ is the current flowing in the $+x$-direction and I_- is the current flowing in the $-x$-direction, then

$$I_+ = 2e \sum_n \int_0^{+\infty} \frac{dk_x}{2\pi} v_x(k_x) f_L(E), \tag{2.169}$$

and

$$I_- = 2e \sum_n \int_{-\infty}^{0} \frac{dk_x}{2\pi} v_x(k_x) f_R(E). \tag{2.170}$$

If we replace $k_x \to -k_y$ in last equation and by using $v_y(-k_x) = -v_y(k_x)$, we have,

$$I_- = -2e \sum_n \int_0^{+\infty} \frac{dk_x}{2\pi} v_x(k_x) f_R(E). \tag{2.171}$$

The total current can be written as,

$$\begin{aligned} I =& I_+ + I_- \\ I =& 2e \sum_n \int_0^\infty \frac{dk_x}{2\pi} v_x(k_x) \left(f_L(E) - f_R(E) \right). \end{aligned} \tag{2.172}$$

Since f depends on k_x through energy, we can replace k_x in the favour of energy by using $dE = \hbar v(k_y) dk$. Thus, we have so-called Landauer formula

$$I = \frac{2e}{2\pi\hbar} \sum_n \int_0^\infty dE \left(f(E - \mu_B) - f(E - \mu_A) \right). \tag{2.173}$$

This is the particular case of the Landauer formula in which $T_n(E) = 1$ or $T_n(E) = 0$. Now let us consider generally we have an ideal waveguide connected with the reservoirs and at the centre we have a scattering region such that any channel have a finite probability of transmission $T_n(E)$ and reflection $R_n(E)$. To calculate the current we take a cross-section located in the left side of the waveguide. The current flowing towards right is,

$$I_L = 2e \sum_n \int_0^\infty \frac{dk_x}{2\pi} v_x(k_x) f_L(E - \mu_L). \tag{2.174}$$

Now the current flowing towards left side contains two parts, a fraction of the originated electrons from left reservoir are reflected, this reflected current can be calculated as,

$$I_{R_1} = 2e \sum_n \int_{-\infty}^0 \frac{dk_x}{2\pi} v_x(k_x) R_n f_L(E - \mu_L), \tag{2.175}$$

and electrons coming from right reservoirs are partially transmitted and partially reflected, hence the second part of the current flowing in the right direction is given by,

$$I_{R_1} = 2e \sum_n \int_{-\infty}^0 \frac{dk_x}{2\pi} v_x(k_x) T_n f_L(E - \mu_R). \tag{2.176}$$

Hence, the total current flowing in the right is,

$$I_R = 2e \sum_n \int_{-\infty}^0 \frac{dk_x}{2\pi} v_x(k_x) \left(R_n f_L(E - \mu_L) + T_n f_L(E - \mu_R) \right). \tag{2.177}$$

Thus, the total current flowing through the cross-section is,

$$I = 2e\sum_n \int_0^\infty \frac{dk_x}{2\pi} v_x(k_x) f_L(E-\mu_L) + 2e\sum_n \int_{-\infty}^0 \frac{dk_x}{2\pi} v_x(k_x)\left(R_n f_L(E-\mu_L) + T_n f_L(E-\mu_R)\right). \tag{2.178}$$

If we replace, $k_x \to -k_x$ in the second part of the above equation and use $v(-k_x) = -v(k_x)$ we obtain,

$$I = 2e\sum_n \int_0^\infty \frac{dk_x}{2\pi} v_x(k_x)\left[(1-R_n(E))f_L(E-\mu_L) - T_n(E) f_R(E-\mu_R)\right]. \tag{2.179}$$

This simplifies into the result,

$$I = 2e\sum_n \int_0^\infty \frac{dk_x}{2\pi} v_x(k_x) T_n(E)\left(f_L(E-\mu_L) - f_R(E-\mu_R)\right). \tag{2.180}$$

If we replace k_x in the favour of energy we obtain the following result,

$$I = \frac{2e}{h}\sum_n \int_0^\infty dE T_n(E)\left(f_L(E-\mu_L) - f_R(E-\mu_R)\right). \tag{2.181}$$

This is the Landauer formulae which converts a conductance problem into one dimensional scattering problem.

Chapter 3

Integer Quantum Hall Effect

3.1 Landau quantization

Here we will discuss the general quantization of kinetic energy of the 2D electron gas. Section (3.1) deals with the wave function of a free particle and how these modify under the influence of a strong magnetic field. The later sections deal with the formalism of these wave function in the symmetric and Landau gauges.

3.1.1 Hamiltonian for a free particle

Hamiltonian for a free particle can be written as,

$$\mathcal{H} = \frac{\mathbf{p}^2}{2m}. \tag{3.1}$$

If we assume mass is isotropic, i.e., the mass of electron in bands is same in all directions, then the Hamiltonian can be written as,

$$\mathcal{H} = \frac{p_x^2}{2m} + \frac{p_y^2}{2m}. \tag{3.2}$$

Here the momentum of electron is constant of motion because, $[\mathbf{p}, \mathcal{H}] = 0$, So the eigenvalues of momentum is a good quantum number in this free particle case.

3.1.2 Hamiltonian with non-zero B-field

The effect of the magnetic field can be easily taken into account by replacing, $\mathbf{P} \to \mathbf{P} - \frac{e}{c}\mathbf{A} \equiv \Pi$, where Π is gauge invariant momentum momentum and $\vec{A}(\vec{r})$ is magnetic vector potential which generates magnetic field according to the equation,

$$\vec{\nabla} \times \mathbf{A} = \mathbf{B}. \tag{3.3}$$

Then the Hamiltonian in (3.2) becomes,

$$\mathcal{H} = \frac{\left(p_x - \frac{e}{c}A_x\right)^2}{2m} + \frac{\left(p_y - \frac{e}{c}A_y\right)^2}{2m}. \tag{3.4}$$

By using the definition of gauge invariant momentum Π, we can write the Hamiltonian as,

$$\mathcal{H} = \frac{\Pi_x^2}{2m} + \frac{\Pi_y^2}{2m}. \tag{3.5}$$

Now the Hamiltonian is not transnationally invariant because, $[\mathbf{P}, \mathcal{H}] \neq 0$.
Let's calculate the commutation relation of Π_x, Π_y,

$$\begin{aligned}
[\Pi_x, \Pi_y] &= \left[\left(p_x - \frac{e}{c}A_x\right), \left(p_y - \frac{e}{c}A_y\right)\right], \\
&= [p_x, p_y] - \frac{e}{c}[p_x, A_y] - \frac{e}{c}[A_x, p_y] + \frac{e^2}{c^2}[A_x, A_y], \\
&= -\frac{e}{c}\left([p_x, A_y] - [p_y, A_x]\right), \\
&= -\frac{e}{c}\left(\frac{\partial A_y}{\partial x}[p_x, x] + \frac{\partial A_y}{\partial y}[p_x, y] - \frac{\partial A_x}{\partial x}[p_y, x] - \frac{\partial A_x}{\partial y}[p_y, y]\right), \\
&= -\frac{e}{c}\left(-i\hbar\frac{\partial A_y}{\partial x} + i\hbar\frac{\partial A_x}{\partial y}\right), \\
&= i\hbar\frac{e}{c}\left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right), \\
&= i\hbar\frac{e}{c}(\nabla \times A) = i\hbar\frac{e}{c}B.
\end{aligned}$$

Defining $l_B = \sqrt{\frac{\hbar c}{eB}}$, where l_B is known as magnetic length, we have,

$$[\Pi_x, \Pi_y] = i\frac{\hbar^2}{l_B^2}. \tag{3.6}$$

This commutation relation allows us to define two very useful operators

$$\begin{aligned} a =& \frac{l_B}{\sqrt{2}\hbar}\left(\Pi_x + i\Pi_y\right), \\ a^\dagger =& \frac{l_B}{\sqrt{2}\hbar}\left(\Pi_x - i\Pi_y\right). \end{aligned} \tag{3.7}$$

The commutation relation between operators defined in (3.9) is,

$$\begin{aligned} \left[a, a^\dagger\right] =& \frac{l_B^2}{2\hbar^2}\left([\Pi_x, \Pi_x] - i[\Pi_x, \Pi_y] + i[\Pi_y, \Pi_x] - i^2[\Pi_y, \Pi_y]\right), \\ =& \frac{l_B^2}{2\hbar^2} 2i[\Pi_x, \Pi_y], \\ \left[a, a^\dagger\right] =& 1. \end{aligned} \tag{3.8}$$

3.1.3 Landau Levels And Energy Eigenvalues

By writing equation (3.176) in terms of Π_x and Π_y we get

$$\begin{aligned} \Pi_x =& \frac{\hbar}{\sqrt{2}l_B}\left(a^\dagger - a\right) \\ \Pi_y =& \frac{\hbar}{\sqrt{2}l_B}\left(a^\dagger + a\right) \end{aligned} \tag{3.9}$$

Using equation (3.9), we can write the Hamiltonian in (3.5) as,

$$\mathcal{H} = \hbar\omega_c\left(a^\dagger a + \frac{1}{2}\right). \tag{3.10}$$

Where $\omega_c = \frac{eB}{mc}$ is cyclotron frequency of electron. Defining $N = a^\dagger a$, where N is a number operator with the following relations,

$$N \mid n\rangle = n \mid n\rangle. \tag{3.11}$$

Where,

$$a^\dagger \mid n\rangle = \sqrt{n+1} \mid n+1\rangle, \quad a \mid n\rangle = \sqrt{n} \mid n-1\rangle. \tag{3.12}$$

If we operate the Hamiltonian on number state we get,

$$\mathcal{H} \mid n\rangle = \hbar\omega_c(n + \frac{1}{2}) \mid n\rangle.$$

Thus the energy eigenvalues labelled by n are given as,

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega_c. \tag{3.13}$$

Thus the motion of an electron in a magnetic field is quantized with the energy levels given by (3.13) similar to the simple harmonic oscillator energy levels.

3.1.4 Wave Functions In Symmetric Gauge

Here we will apply the formalism developed in the previous section to find the wave function of an electron in a strong magnetic field and represent them in the complex notation. To accomplish this, we need to define a gauge which generates the magnetic field. Let's assume that the magnetic field is frozen along $z - axis$. The magnetic vector potential in symmetric gauge is,

$$\vec{A} = \left(-\frac{B}{2}y, \frac{B}{2}x\right). \tag{3.14}$$

This gauge is also called rotational invariant gauge. It can easily be verified that $\vec{\nabla} \times \vec{A} = B\hat{z}$, for this gauge. In this gauge the component of gauge invariant momentum are,

$$\begin{aligned} \Pi_x =& p_x + \frac{eB}{2c}y, \\ \Pi_y =& p_y - \frac{eB}{2c}x. \end{aligned} \tag{3.15}$$

To find the ground state Ψ_0, we use,

$$\hat{a}\Psi_0 = 0. \tag{3.16}$$

Since $\hat{a}$ is lowering operator, it kills the ground state. First, let us find the complex notation for $\hat{a}$ defined in (3.7),

$$\begin{aligned}
\hat{a} =& \frac{l_B}{\sqrt{2}\hbar}\left(\Pi_x + i\Pi_y\right), \\
=& \frac{l_B}{\sqrt{2}\hbar}\left(p_x + \frac{eB}{2c}y + ip_y - i\frac{eB}{2c}x\right), \\
=& \frac{l_B}{\sqrt{2}\hbar}\left(p_x + ip_y + \frac{eB}{2c}x - i\frac{eB}{2c}x\right), \\
=& -i\frac{l_B}{\sqrt{2}}[(\nabla_x + i\nabla_y) + \frac{eB}{2\hbar c}(x+iy)], \\
\hat{a} =& -i\sqrt{2}l_B\left(\overline{\partial} + \frac{eB}{4\hbar c}z\right).
\end{aligned} \tag{3.17}$$

Now apply $\hat{a}$ on the ground state Ψ_0.

$$\hat{a}\Psi_0 = 0, \tag{3.18}$$

$$-i\sqrt{2}l_B\left(\overline{\partial} + \frac{eB}{4\hbar c}z\right)\Psi(z,\overline{z}) = 0, \Rightarrow \Psi(z,\overline{z}) = N_m z^m \exp\left(-\frac{eB}{2\hbar c}z\overline{z}\right), \tag{3.19}$$

$$\Psi_{0,m} = N_m z^m \exp\left(-\frac{eB}{2\hbar c}z\overline{z}\right), \tag{3.20}$$

N_m can be evaluated by using normalization condition.

3.1.5 Level degeneracy

Our original Hamiltonian has two pairs of conjugate operators, x and p_x, and y and p_y. When we express the Hamiltonian in the form of ladder operators (3.9) we have one pair of conjugate operator $\hat{a}$ and $\hat{a}^\dagger$. The search for the other conjugate pair gives rise to level degeneracy.

Within the classical treatment, symmetric gauge allows us to make a connection with classical constant of motion that one obtains by solving classical equations of motion for the massive electrons in a magnetic field.

$$\begin{aligned}
m\ddot{r} &= e(\dot{r} \times B), \\
\Rightarrow \ddot{x} = \omega_c\dot{x}, &\quad \ddot{y} = -\omega_c\dot{y}.
\end{aligned} \tag{3.21}$$

The above equations describe acceleration due to Lorentz force. By integrating with respect to time we get,

$$\begin{cases} x = X + \frac{\Pi_y}{m\omega_c}, \\ y = Y - \frac{\Pi_x}{m\omega_c}. \end{cases} \tag{3.22}$$

Here $R = (X, Y)$ are the integration constant. In the semi-classical treatment these are the guiding-centre operators for the electron's cyclotron motion, given as,

$$\begin{aligned} X &= x - \frac{\Pi_y}{m\omega_c}, \\ Y &= y + \frac{\Pi_x}{m\omega_c}. \end{aligned} \tag{3.23}$$

The commutation relation between these guiding centre operators is,

$$[X, Y] = \left[x - \frac{\Pi_y}{m\omega_c}, y + \frac{\Pi_x}{m\omega_c}\right] = -il_B^2. \tag{3.24}$$

This commutation relation allows us to define two operators,

$$\begin{aligned} b &= \frac{1}{\sqrt{2}l_B}(X - iY), \\ b^\dagger &= \frac{1}{\sqrt{2}l_B}(X + iY). \end{aligned} \tag{3.25}$$

The commutation relation between the operator defined in (3.25) is,

$$[b, b^\dagger] = \frac{1}{2l_B^2}\{i[X, Y] - i[Y, X]\} = \frac{1}{2l_B^2}\left(l_B^2 + l_B^2\right) = 1.$$

The complex representation of these operators is given by,

$$\begin{aligned} b &= \frac{\hbar\sqrt{2}}{m\omega_c l_B}\left(\partial + \frac{eB}{4\hbar c}\overline{z}\right), \\ b^\dagger &= \frac{\hbar\sqrt{2}}{m\omega_c l_B}\left(-\overline{\partial} + \frac{eB}{4\hbar c}z\right). \end{aligned} \tag{3.26}$$

Let's check the action of $b^\dagger$ on the $\Psi_{0,0}$,

$$b^\dagger\Psi_{0,0} = \frac{\hbar\sqrt{2}}{m\omega_c l_B}\left(-\overline{\partial} + \frac{eB}{4\hbar c}z\right)\Psi_{0,0} = Nz\exp\left(-\frac{z\overline{z}}{4\hbar c}\right)s = \Psi_{0,1}.$$

Hence $b^\dagger$ is an operator which generates all ground states. By consecutive application of $b^\dagger$ we have,

$$\left(b^\dagger\right)^m \Psi_{0,0} = \Psi_{0,m}. \tag{3.27}$$

So b and $b^\dagger$ behave as creation and annihilation operators. The action of $a^\dagger$ on ground state is,

$$a^\dagger \Psi_{0,0} = \Psi_{1,0}.$$

Hence,

$$\left(a^\dagger\right)^n \left(b^\dagger\right)^m \Psi_{0,0} = \Psi_{n,m}.$$

Hence, for each value of n there are infinite values of m. Each Landau Level is infinitely degenerate. Now we find the restriction on the values of m. For ground state $n = 0$, the probability density for the ground state is,

$$\mid \Psi_{0,m} \mid^2 = \mid N_m \mid^2 z^{2m} \exp\left(-\frac{eB}{2\hbar c} \mid z \mid^2\right).$$

The probability density is shaped like a ring around the origin. To find r_{max},

$$\frac{dP}{dr} = 0 = 2\pi N^2 \left((2m+1)\, r^{2m} - \frac{eB}{\hbar c} r^{2m+2}\right),$$
$$r_{max}^2 = (2m+1)\,\frac{\hbar c}{eB}.$$

Consider R is the radius of ring such that

$$r_{max}^2 \leq R^2 \tag{3.28}$$
$$(2m+1)\,\frac{\hbar c}{eB} \leq R^2,$$
$$m \leq \frac{eBR^2}{2\hbar c} = \frac{\Phi}{hc/e} = \frac{\Phi}{\Phi_0}. \tag{3.29}$$

Here $\Phi_0 = hc/e$ is called flux quantum. So maximum number of states depends upon the ratio of magnetic flux threading through the sample to the flux quantum.

3.1.6 Wave functions in Landau Gauge

If the sample geometry is rectangular the Landau gauge, $\mathbf{A}(\mathbf{r}) = (-y, 0, 0)$ is more appropriate. In this gauge the Hamiltonian is translationally invariant in the x-direction, so $p_x = \hbar k$ is a good quantum number. The Hamiltonian (3.2)

becomes,

$$\mathcal{H} = \frac{\left(p_x - \frac{eB}{c}y\right)^2}{2m} + \frac{p_y^2}{2m}. \tag{3.30}$$

We can make a plane wave ansatz,

$$\Psi_{n,k}(x,y) = \frac{\exp(ikx)}{\sqrt{L}}\chi_{n,k}(y).$$

The Hamiltonian becomes,

$$\mathbf{H} = \frac{p_y^2}{2m} + \frac{1}{2}m\omega_c^2\left(y - y_0\right)^2. \tag{3.31}$$

This is the Hamiltonian of a harmonic oscillator centred about point $y_0 = kl_B^2$. The solution of the Schrodinger's equation is,

$$\Psi_{n,k}(x,y) = \frac{\exp(ikx)}{\sqrt{L}}H_n\left(\frac{y - y_0}{l_B}\right)\exp\left(-\frac{\left(y - y_0\right)^2}{4l_B^2}\right). \tag{3.32}$$

Periodic boundary conditions along x direction quantize k, as $k = m \times 2\pi/L$. The maximum number of states can be determined as discussed previously by

$$M = \frac{\Phi}{\Phi_0}. \tag{3.33}$$

For each value of n there are M number of degenerate states. So each Landau level has M degenerate states.

3.2 Edge Currents and conductivity

3.2.1 Ideal perfect conductor

Consider an ideal perfect conductor without impurities or inhomogeneities of width W connecting two electron reservoirs as shown in fig(3.1). The electron reservoirs, at chemical potentials μ_L and μ_R, act as source or sink of energy and carriers. Every reservoir eject electrons into current carrying states upto its chemical potential.

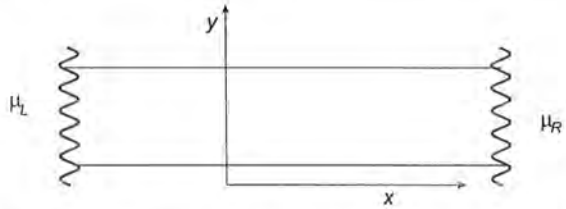

FIGURE 3.1: Perfect two-dimensional conductor connected to reservoirs. The chemical potentials are μ_L and μ_R.

3.2.1.1 B = 0 case

Now consider the Hamiltonian for zero magnetic field with a potential along the y-direction,

$$\mathcal{H} = \frac{p_x^2}{2m} + \left(\frac{p_y^2}{2m} + V(y)\right). \tag{3.34}$$

The wave functions are separable and labelled by n and k. The sample has finite length L along x-direction and width W along y direction. The x-direction motion is free particle motion. The wave function then can be written as,

$$\Psi_{n,k} = \exp(ikx)\, f_{n,k}(y).$$

The application of the Hamiltonian (3.34) on $\Psi n, k$ gives,

$$\left(\frac{p_x^2}{2m} + V(y) + \frac{\hbar^2 k^2}{2m}\right) f_{n,k}(y) = \epsilon_{n,k} f_{n,k}(y),$$

$$\epsilon_{n,k} = \frac{\hbar^2 k_n^2}{2m} + E_n. \tag{3.35}$$

Here the periodic boundary conditions yields the quantization of k with E_n being the energy of transverse motion. Now let's calculate the current using the Landauer formula in equation (2.181) for the current of a single conducting state,

$$I_n = \frac{e}{h}\int d\varepsilon \left(f_F(\varepsilon - \mu_L) - f_F(\varepsilon - \mu_L)\right). \tag{3.36}$$

We use here $T_n(\varepsilon) = 1$, for the perfect conductor. The Fermi distribution function is given by,

$$f_F(\varepsilon - \mu) = \frac{1}{\exp\left(\frac{\varepsilon-\mu}{kT}\right) + 1}. \tag{3.37}$$

At low temperature, we can write,

$$f_F(\varepsilon - \mu_L) - f_F(\varepsilon - \mu_R) = \frac{\partial f}{\partial \varepsilon} \times (\mu_L - \mu_R).$$

Then the current (3.36) becomes,

$$I_n = \frac{e}{h}\left[\int d\varepsilon \times \frac{\partial f}{\partial \varepsilon}\right](\mu_L - \mu_R). \tag{3.38}$$

In IQHE, we take $T = 0$. Therefore, f becomes a step function and derivative of f with respect to energy is a delta function around Fermi energy, i.e.,

$$\frac{\partial f}{\partial \varepsilon} = \delta(\varepsilon - \varepsilon_F). \tag{3.39}$$

Hence, the integral (3.38) becomes,

$$I_n = \frac{e}{h}\Delta\mu.$$

This shows that the current does not depend upon index n. Each filled Landau level contributes the same amount of current. Suppose the Fermi level lies midway between the nth and $n+1^{th}$ level, then there are n completely filled Landau levels which contribute to current. So the total current becomes,

$$I_{tot} = n\frac{e}{h}(\mu_L - \mu_R).$$

The voltage drop between the reservoirs is, $\Delta\mu = eV$. Hence, the total current becomes,

$$I_{tot} = n\frac{e^2}{h} \times V.$$

The conductivity is then becomes,

$$\sigma_{xy} = n\frac{e^2}{h}. \tag{3.40}$$

3.2.2 Non-zero B field

Now let us consider an ideal perfect conductor placed in a magnetic field which points in the z-direction. This ideal perfect conductor has length L and width W where W is much less than length L. Electrons are confined in this rectangular geometry by using a potential $V_{conf}(y)$ that only depends upon y and the system remains translationally invariant in the x-direction. We take the magnetic vector potential, $\mathbf{A} = (-By, 0, 0)$. The Hamiltonian then becomes,

$$\mathcal{H} = \frac{\left(p_x + \frac{eB}{c}y\right)^2}{2m} + \frac{p_y^2}{2m} + V_{conf}(y). \tag{3.41}$$

Where $V_{conf}(y) = 0$, inside the sample and increases rapidly near the edges. For inside the sample the Hamiltonian is,

$$\mathcal{H} = \frac{\left(p_x + \frac{eB}{c}y\right)^2}{2m} + \frac{p_y^2}{2m}.$$

The eigenvalue equation is,

$$\mathcal{H}\Psi = \varepsilon\Psi.$$

The wave function can be decomposed due to translational invariance of Hamiltonian in the x-direction as,

$$\Psi_{n,k}(x,y) = \frac{\exp(ikx)}{\sqrt{L}} f_{n,k}(y). \tag{3.42}$$

The application of the Hamiltonian on the wave function (3.42) gives us

$$\begin{aligned}
&\left(\frac{\left(p_x + \frac{eB}{c}y\right)^2}{2m} + \frac{p_y^2}{2m}\right)\Psi_{n,k}(x,y) = \varepsilon_{n,k}\Psi_{n,k}(x,y),\\
&\left(\frac{\left(\hbar k + \frac{eB}{c}y\right)^2}{2m} + \frac{p_y^2}{2m}\right) f_{n,k}(y) = \varepsilon_{n,k} f_{n,k}(y),\\
&\left(\frac{1}{2m} \times \frac{e^2B^2}{c^2}\left(y + \frac{\hbar c}{eB}k\right) + \frac{p_y^2}{2m}\right) f_{n,k}(y),\\
&\left(\frac{p_y^2}{2m} + \frac{1}{2}m\omega_c^2\left(y - y_0\right)^2\right) f_{n,k}(y) = \varepsilon_{n,k} f_{n,k}(y).
\end{aligned} \tag{3.43}$$

This is the equation of a Harmonic Oscillator with shifted centre, where

$$l_B^2 = \frac{\hbar c}{eB}, \tag{3.44}$$

and

$$y_0 = -kl_B^2. \tag{3.45}$$

The solution of equation (3.43) is,

$$f_{n,k} = H_n\left(y - y_0\right)\exp\left(-\frac{\left(y - y_0\right)^2}{4l_B^2}\right).$$

So the complete wave function becomes,

$$\Psi_{n,k}(x,y) = \frac{\exp(ikx)}{\sqrt{L}} H_n\left(y - y_0\right)\exp\left(-\frac{\left(y - y_0\right)^2}{4l_B^2}\right). \tag{3.46}$$

The energy eigenvalues in this case can be written as,

$$\varepsilon_{n,k} = \left(n + \frac{1}{2}\right)\hbar\omega_c. \tag{3.47}$$

Now let there be a confinement potential. This leads to an eigenvalue problem for the function $f_{n,k}$,

$$\varepsilon_{n,k} f_{n,k} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{1}{2}m\omega_c^2\left(y - y_0\right) + V_{conf}(y)\right] f_{n,k}. \tag{3.48}$$

The confinement potential varies strongly near the sample edges, i.e., in the vicinity of y_1 and y_2. We assume adiabatic variation, i.e., the potential varies strongly with respect to the dimension of the sample but does not vary much compare to the magnetic length l_B. For a fixed value of k, y_0 is fixed. So we can expand the potential about y_0 and by ignoring the second order terms we get,

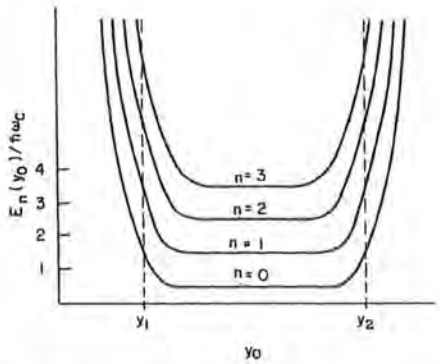

FIGURE 3.2: Perfect two-dimensional conductor connected to reservoirs. The chemical potentials are μ_L and μ_R.

$$V(y) = V(y_0) + (y - y_0)\frac{\partial V}{\partial y}\,|_{y=y_0}\,.$$

We define here local electric field in terms of the first derivative of potential at y_0,

$$eE(y_0) = \frac{\partial V}{\partial y}\,|_{y=y_0}\,.$$

Using this, the expansion of potential in first order becomes,

$$V(y) = V(y_0) - (y - y_0)eE(y_0).$$

The operator part of the equation (3.48) is,

$$\begin{aligned}
&\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}+\frac{1}{2}m\omega_c^2\left(y-y_0\right)+V_{conf}(y)\right],\\
&=\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}+\frac{1}{2}m\omega_c^2\left(y-y_0\right)^2+V(y_0)-(y-y_0)eE(y_0)\right],\\
&=\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}+\frac{1}{2}m\omega_c^2\left(\left(y-y_0\right)^2-\frac{2E(y_0)}{m\omega_c^2}\left(y-y_0\right)\right)+V(y_0)\right],\\
&=\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}+\frac{1}{2}m\omega_c^2\left(\left(y-y_0\right)^2-\frac{2eE(y_0)}{m\omega_c^2}\left(y-y_0\right)+\left(\frac{eE(y_0)}{m\omega_c^2}\right)^2-\left(\frac{eE(y_0)}{m\omega_c^2}\right)^2\right)+V(y_0)\right],\\
&=\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}+\frac{1}{2}m\omega_c^2\left(y-y\prime_0\right)^2-\frac{1}{2}mv_D^2+V(y_0)\right].
\end{aligned} \tag{3.49}$$

Here,

$$v_D=\frac{E(y_0)}{B}, \tag{3.50}$$

is the drift velocity and the position of the centre of the harmonic oscillator is shifted from $y_0 \to y_0' = y_0 + eE(y_0)/m\omega_c^2$. We can see that the drift velocity term in the above expansion has to be dropped as it is second order in electric field. This leads to the result,

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}+\frac{1}{2}m\omega_c^2\left(y-y_0\right)+V_{conf}(y)\right]=\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}+\frac{1}{2}m\omega_c^2\left(y-y\prime_0\right)^2+V_{conf}(y_0)\right]. \tag{3.51}$$

Hence, the eigenvalue equation (3.48) becomes,

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}+\frac{1}{2}m\omega_c^2\left(y-y\prime_0\right)^2+V_{conf}(y_0)\right]f_{n,k}=\varepsilon_{n,k}f_{n,k}. \tag{3.52}$$

The energy eigenvalues becomes,

$$\varepsilon_{n,y_0}=\left(n+\frac{1}{2}\right)\hbar\omega_c+V_{conf}(y_0). \tag{3.53}$$

Here prime is omitted to keep the notation simple. This is the same energy spectrum as without confinement potential apart from a potential term at the centre of the position of harmonic oscillator which may indeed vary strongly. For hard well potential the energy spectrum shown in fig.(3.2).

Periodic boundary conditions allows us to apply arguments similar to Bloch functions, one can show that the carrier velocity at the edge state is,

$$v_{nk} = \langle nk|v_x|nk\rangle = \frac{1}{\hbar}\frac{d\varepsilon_n}{dk} = \frac{1}{\hbar}\frac{d\varepsilon_{ny_0}}{dy_0}\frac{dy_0}{dk}.$$

From equation (3.45) the derivative of y_0 is,

$$\frac{dy_0}{dk} = -l_B^2. \tag{3.54}$$

Hence, the velocity of the carrier in the edge state is given by,

$$v_{nk} = -\frac{l_B^2}{\hbar}\frac{d\varepsilon_{ny_0}}{dk}. \tag{3.55}$$

Thus the velocity of the carriers in an edge state is proportional to the Landau level. The velocity is negative at the lower edge y_1 and positive at the upper edge y_2. Note that the velocity is zero in the bulk Landau states where ε_{ny_0} is independent of y_0. The magnetic field quenches the kinetic energy for longitudinal motion. The density of states along a Landau level approximately for one dimensional conductors is given by,

$$\frac{dN}{dk} = \frac{1}{2\pi}.$$

Further the density of the states is related to the velocity of the carriers in an edge state as,

$$\left[\frac{dN}{d\varepsilon}\right]_n = \frac{dN}{dk}\left[\frac{dk}{d\varepsilon}\right]_n = \frac{1}{2\pi\hbar v_{nk}}. \tag{3.56}$$

The no of states at Fermi energy (i.e., the number of the values of the k) determined by the equation,

$$E_F = \varepsilon_{ny_0} = (n + \frac{1}{2})\hbar\omega_c + V_{conf}(y_0). \tag{3.57}$$

The current fed into each edge state is as calculated in zero-B field case, discussed previously,

$$I_n = ev_n\left[\frac{dN}{d\varepsilon}\right]_n(\mu_1 - \mu_2) = \frac{e}{h}\Delta\mu.$$

The current fed in each channel is independent from n. So for n completely filled channels the total current is,

$$I_{tot} = n\frac{e}{h}\Delta\mu. \tag{3.58}$$

Thus the current fed into an edge state by a reservoir is the same as the current fed into a quantum channel in a zero-field perfect conductor. The resulting

conductivity is again found to be the same as for zero-field case, i.e.,

$$\sigma_{xy} = \frac{e^2}{h} n. \tag{3.59}$$

3.3 Gauge invariant and quantization of Hall conductance

Here, we will discuss the different aspects of the wave function of electrons in a perpendicular magnetic field with the periodic potential. We review here some basic properties of the Bloch electrons and we calculate the Hall conductance by the Kubo formulae in the linear response. We will show that the Hall conductance is a gauge invariant quantity. This argument leads to quantization of conductivity.

3.3.1 Bloch electron in magnetic field

The Hamiltonian for a two dimensional electron gas subjected to a perpendicular magnetic field is,

$$\mathcal{H} = \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 + U(x, y). \tag{3.60}$$

Where, $U(x, y)$ is a periodic potential in both dimensions, i.e.,

$$U(x + a, y) = U(x, y),$$
$$U(x, y + b) = U(x, y).$$

This shows that the system is invariant under these translation but the Hamiltonian is not because the Hamiltonian contains a gauge dependent quantity $\mathbf{A}$, which depends upon the position although the magnetic field is not. We need to choose an appropriate gauge to make Hamiltonian translationally invariant under these translations. Let $\mathbf{R}$ is Bravais lattice vector, i.e.,

$$\mathbf{R} = n\mathbf{a} + m\mathbf{b}. \tag{3.61}$$

Here n and m are integers. We know that an ordinary translation operator is,

$$T_R = \exp\left(\frac{i}{\hbar}\mathbf{R} \cdot \mathbf{p}\right). \tag{3.62}$$

This translation operator acts on any smoothly varying function $f(\mathbf{r})$ and gives,

$$T_{\vec{R}} f(\mathbf{r}) = f(\mathbf{r} + \mathbf{R}). \tag{3.63}$$

Let us choose the symmetric gauge, i.e.,

$$\mathbf{A} = \frac{1}{2}(\mathbf{B} \times \mathbf{r}). \tag{3.64}$$

We can easily verify that,

$$\vec{\nabla} \times \mathbf{A} = B\hat{z}. \tag{3.65}$$

The magnetic translation operator in the symmetric gauge is,

$$\hat{T}_{\vec{R}} = e^{\frac{i}{\hbar}\mathbf{R}\cdot\left(\mathbf{p} - \frac{e}{2c}(\mathbf{B}\times\mathbf{r})\right)}. \tag{3.66}$$

In terms of an ordinary translational operator, we can write this,

$$\hat{T}_{\vec{R}} = T_{\vec{R}} e^{\frac{-ie}{\hbar c}\frac{(\mathbf{B}\times\mathbf{R})\cdot\mathbf{r}}{2}}. \tag{3.67}$$

If we apply $T_{\vec{R}}$ on the Hamiltonian (3.60), it left $U(\vec{r})$ invariant. However, the magnetic vector potential is transformed to $\mathbf{A}(\vec{r} + \vec{R})$. In general,

$$\mathbf{A}(\vec{r} + \vec{R}) \neq \mathbf{A}(\vec{r}). \tag{3.68}$$

Since, the magnetic field is uniform. Thus, $\mathbf{A}(\vec{r})$ and $\mathbf{A}(\vec{r} + \vec{R})$ differ by a gradient of a scalar function, i.e.,

$$\mathbf{A}(\vec{r}) = \mathbf{A}(\vec{r} + \vec{R}) + \vec{\nabla} g. \tag{3.69}$$

In the symmetric gauge,

$$\mathbf{A}(\mathbf{r} + \mathbf{R}) = \frac{1}{2}(\mathbf{B} \times \mathbf{r}) - \vec{\nabla} g. \tag{3.70}$$

Where the ∇g is defined as,

$$\vec{\nabla} g = \frac{1}{2}(\mathbf{B} \times \mathbf{R}). \tag{3.71}$$

Now we show that the magnetic translation operator defined in (3.66) commutes with the Hamiltonian (3.60). Consider, $f(\mathbf{r})$ is any smoothly varying function such

that

$$\hat{T}_{\vec{R}}\mathcal{H}f(\mathbf{r}) = e^{\frac{-ie}{\hbar c}\frac{(\mathbf{B}\times\mathbf{R})\cdot\mathbf{r}}{2}}\frac{1}{2m}\left(\mathbf{p}-\frac{e}{2c}\mathbf{B}\times\mathbf{r}-\frac{e}{2c}\mathbf{B}\times\mathbf{R}\right)^2 f(\mathbf{r}+\mathbf{R}). \tag{3.72}$$

On the other hand,

$$\mathcal{H}\hat{T}_{\vec{R}}f(\mathbf{r}) = \frac{\left(\mathbf{p}-\frac{e}{2c}\mathbf{B}\times\mathbf{r}\right)^2}{2m}\exp\frac{-ie}{\hbar c}\frac{(\mathbf{B}\times\mathbf{R}).\mathbf{r}}{2}T_{\vec{R}}f(\mathbf{r}). \tag{3.73}$$

By operating sequentially we get,

$$\mathcal{H}\hat{T}_{\mathbf{R}} = \exp\left(\frac{-ie}{\hbar c}\frac{(\mathbf{B}\times\mathbf{R}).\mathbf{r}}{2}\right)\frac{1}{2m}\left(\mathbf{p}-\frac{e}{2c}\mathbf{B}\times\mathbf{r}-\frac{e}{2c}\mathbf{B}\times\mathbf{R}\right)^2 f(\mathbf{r}+\mathbf{R}) = \hat{T}_{\vec{R}}\mathcal{H}f(\mathbf{r}). \tag{3.74}$$

This shows that the Hamiltonian is invariant under the translation $\hat{T}_{\vec{R}}$, i.e.,

$$[\hat{T}_{\vec{R}}, \mathcal{H}] = 0. \tag{3.75}$$

Now, we have to work out the commutation relation between the magnetic translation operators with each other, for simplicity we choose,

$$\mathbf{R}_a = a\hat{x}, \qquad \mathbf{R}_b = b\hat{y}, \qquad \mathbf{r} = x\hat{x}+y\hat{y}. \tag{3.76}$$

So,

$$\begin{aligned}\hat{T}_a &= \exp\left(-i\frac{eBa}{2\hbar c}y\right)T_a,\\ \hat{T}_b &= \exp\left(i\frac{eBb}{2\hbar c}x\right)T_b.\end{aligned} \tag{3.77}$$

Let us apply these operators on any smoothly varying function $f(\mathbf{r})$, we get,

$$\hat{T}_a\hat{T}_b f(\mathbf{r}) = \exp\left(i\pi\frac{\Phi}{\Phi_0}\right)\exp\left(-i\frac{eBa}{2\hbar c}y\right)\exp\left(i\frac{eBb}{2\hbar c}x\right)f(\mathbf{r}+a\hat{x}+b\hat{y}). \tag{3.78}$$

Here we define, $\Phi = Bba$ the flux threading through a magnetic unit cell and Φ_0 is the usual flux quantum. Similarly,

$$\hat{T}_b\hat{T}_a f(\mathbf{r}) = \exp\left(-i\pi\frac{\Phi}{\Phi_0}\right)\exp\left(-i\frac{eBa}{2\hbar c}y\right)\exp\left(i\frac{eBb}{2\hbar c}x\right)f(\mathbf{r}+a\hat{x}+b\hat{y}). \tag{3.79}$$

Above equations (3.78) and (3.79) imply that,

$$\hat{T}_a\hat{T}_b = \hat{T}_b\hat{T}_a\exp\left(i2\pi\phi\right). \tag{3.80}$$

Here we define,

$$\phi = \frac{\Phi}{\Phi_0}, \tag{3.81}$$

magnetic flux number in the unit cell. Note that: the magnetic translation operators do not commute with each in general because ϕ may be a rational number. Suppose ϕ is a rational number such that

$$\phi = \frac{p}{q}, \tag{3.82}$$

where p and q are relative prime. We can construct a subset of translations which commute with each other. We take a large unit cell which an integral multiple of flux goes through. Suppose, the Bravais lattice vectors of the form,

$$\vec{R'} = n(q\vec{a}) + m\vec{b}, \tag{3.83}$$

are taken. Then, p magnetic flux quanta are in the magnetic unit cell of area $(qa)b$, and

$$\hat{T}_{\vec{R_1'}}\hat{T}_{\vec{R_2'}} = \hat{T}_{\vec{R_2'}}\hat{T}_{\vec{R_1'}}, \tag{3.84}$$

also,

$$\hat{T}_{\vec{R_1'}}\hat{T}_{\vec{R_2'}} = \hat{T}_{\vec{R_1'}+\vec{R_2'}}. \tag{3.85}$$

Now consider $\Psi(x, y)$ is common eigenstate of $\hat{T}_{\mathbf{R}'}$ and $\mathcal{H}$. The eigenvalues of $\hat{T}_{qa}$ and $\hat{T}_b$ are given by,

$$\begin{aligned} \hat{T}_{qa}\Psi(x, y) &= \exp\left(ik_x qa\right)\Psi(x, y), \\ \hat{T}_b\Psi(x, y) &= \exp\left(ik_y b\right)\Psi(x, y), \end{aligned} \tag{3.86}$$

where k_x and k_y are crystal momentum in respective directions. The magnetic Brillouin zone is,

$$\begin{aligned} 0 \leq k_x &\leq \frac{2\pi}{qa}, \\ 0 \leq k_y &\leq \frac{2\pi}{b}. \end{aligned} \tag{3.87}$$

The eigenstates are labelled by k_x and k_y in addition with band index n, the eigenstate can be written as,

$$\Psi^{(n)}_{k_x,k_y}(x, y) = \exp i\left(k_x x + k_y y\right) u^{(n)}_{k_x,k_y}(x, y). \tag{3.88}$$

By applying $\hat{T}_{qa}$ on $\Psi^{(n)}_{k_x,k_y}(x,y)$ and using (3.77) we get,

$$\hat{T}_{qa}\Psi^{(n)}_{k_x,k_y}(x,y) = \exp\left(-i\frac{eBaq}{2\hbar c}y\right)\exp i\left(k_x(x+qa)+k_y y\right)u^{(n)}_{k_x+qa,k_y}(x+qa,y),$$

$$\Rightarrow \quad u^{(n)}_{k_x,k_y}(x+qa,y) = \exp\left(i\frac{\pi y p}{p}\right)u^{(n)}_{k_x,k_y}(x,y). \tag{3.89}$$

Similarly,

$$u^{(n)}_{k_x,k_y}(x,y+b) = \exp\left(-i\frac{\pi}{a}x\frac{p}{q}\right)u^{(n)}_{k_x,k_y}(x,y). \tag{3.90}$$

These are the generalised Bloch conditions on $u^{(n)}_{k_x,k_y}(x,y)$. Note that: going backwards changes the sign in exponential, i.e.,

$$u^{(n)}_{k_x,k_y}(x-qa,y) = \exp\left(-i\frac{\pi y p}{p}\right)u^{(n)}_{k_x,k_y}(x,y),$$

$$u^{(n)}_{k_x,k_y}(x,y-b) = \exp\left(i\frac{\pi}{a}x\frac{p}{q}\right)u^{(n)}_{k_x,k_y}(x,y). \tag{3.91}$$

This implies that going one way around the magnetic unit cell accumulate net phase $-2\pi p$. Let,

$$u_{k_x,k_y}(x,y) = \mid u_{k_x,k_y}(x,y) \mid \exp(i\theta(x,y)). \tag{3.92}$$

This implies that by integrating over a closed loop in counter clockwise direction, we obtain,

$$-2\pi p = \oint d\ell \cdot \vec{\nabla}_\ell \theta. \tag{3.93}$$

Here,

$$\vec{\nabla}_\ell \theta = \frac{\partial\theta(x,y)}{\partial\ell}. \tag{3.94}$$

We omit here the band index n to keep the notation simple.

3.3.2 Linear response formula and Hall conductance

The Schrdinger equation is,

$$\mathcal{H}\Psi = \varepsilon\Psi. \tag{3.95}$$

By replacing the Hamiltonian (3.60), we get,

$$\left[\frac{1}{2m}\left(\mathbf{p}-\frac{e}{c}\mathbf{A}\right)^2 + U(x,y)\right]\exp(i\vec{k}\cdot\vec{r})u^{(n)}_{k_x k_y} = \varepsilon^{(n)}\exp(i\vec{k}\cdot\vec{r})u^{(n)}_{k_x k_y}. \tag{3.96}$$

It is useful to write above equation as,

$$\left[\frac{1}{2m}\left(\mathbf{p}+\hbar\mathbf{k}-e\frac{A}{c}\right)+U(x,y)\right]u^{(n)}_{k_xk_y}=\varepsilon^{(n)}u^{(n)}_{k_xk_y}. \tag{3.97}$$

Hence, the $\vec{k}$ dependent Hamiltonian can be read as,

$$\hat{\mathcal{H}}(k_x,k_y)=\frac{1}{2m}\left(\mathbf{p}+\hbar\mathbf{k}-e\frac{A}{c}\right)+U(x,y). \tag{3.98}$$

Where k_x and k_y are component of $\vec{k}$ along x- and y-directions respectively. Note that: the eigenvalues $\varepsilon^{(n)}$ depend continuously on $\vec{k}$. In a fixed band n, different values of $\varepsilon^{(n)}$ corresponds to different values of $\vec{k}$ form a magnetic sub-band. When we apply small electric field, this field draws the current through thee sample. We can calculate this current by Nakano-Kubo formula. In linear response theory, the Kubo formula for Hall conductance is,

$$\sigma_{xy}=ie^2\hbar\sum_{\varepsilon_n<\varepsilon_F<\varepsilon_m}\frac{\langle n|v_y|m\rangle\langle n|v_x|m\rangle-\langle n|v_x|m\rangle\langle n|v_y|m\rangle}{(\varepsilon_n-\varepsilon_m)^2}. \tag{3.99}$$

Where ε_F is Fermi energy. The sum is over all states below and above the Fermi energy. The indices n and m represents band index. We also need $\vec{k}$ to specify a state with band index. The presence of $\vec{k}$ must be clicked whenever the band index present. The velocity operator from Heisenberg equation of motion is,

$$\vec{v}=\frac{1}{m}\left(\vec{p}-\frac{e}{c}\vec{A}\right). \tag{3.100}$$

The states are normalised as,

$$\int_0^{qa}dx\int_0^b dy u^{(n)}_{k_xk_y}u^{(m)}_{k'_xk'_y}=\delta^{nm}\delta_{k_xk'_x}\delta_{k_yk'_y}. \tag{3.101}$$

The velocity operator (3.100) can be replaced by partial derivative of the $\vec{k}$ dependent Hamiltonian, i.e.,

$$v_x=\frac{\partial\hat{\mathcal{H}}(k_x,k_y)}{\hbar\partial k_x}=\frac{1}{m}\left(p_x+\hbar k_x-\frac{e}{c}A_x\right). \tag{3.102}$$

Note that here k_x gives no contribution to the current because,

$$\langle m|k_x|n\rangle=0. \tag{3.103}$$

Here we are taking off-diagonal component for which, $m \neq n$. Therefore,

$$\langle n|v_x|m\rangle = \frac{1}{\hbar}\langle n|\partial\frac{\hat{\mathcal{H}}}{\partial k_x}|m\rangle. \tag{3.104}$$

Consider,

$$\frac{\partial}{\partial k_x}\langle n|\hat{\mathcal{H}}|m\rangle = \varepsilon_m\frac{\partial}{\partial k_x}\langle n|m\rangle = 0,$$

$$\langle\frac{\partial n}{\partial k_x}|\hat{\mathcal{H}}|m\rangle + \langle n|\frac{\partial\hat{\mathcal{H}}}{\partial k_x}|m\rangle + \langle n|\hat{\mathcal{H}}|\frac{\partial m}{\partial k_x}\rangle = 0. \tag{3.105}$$

$$\tag{3.106}$$

This gives us a very useful result,

$$\langle n|\frac{\partial\hat{\mathcal{H}}}{\partial k_x}|m\rangle = (\varepsilon_m - \varepsilon_n)\langle n|\frac{\partial m}{\partial k_x}\rangle, \tag{3.107}$$

or,

$$\langle n|\frac{\partial\hat{\mathcal{H}}}{\partial k_x}|m\rangle = -(\varepsilon_m - \varepsilon_n)\langle\frac{\partial n}{\partial k_x} \mid m\rangle. \tag{3.108}$$

The expression for conductivity (3.99) becomes,

$$\sigma_{xy} = \frac{ie^2}{\hbar A}\sum_{\varepsilon_n<\varepsilon_F<\varepsilon_m}\left(\langle\frac{\partial n}{\partial k_x} \mid m\rangle\langle m \mid \frac{\partial n}{\partial k_y} + \langle\frac{\partial m}{\partial k_x} \mid n\rangle\langle n \mid \frac{\partial m}{\partial k_y}\rangle\right). \tag{3.109}$$

Using the identity,

$$\sum_{\varepsilon_n<\varepsilon_F<\varepsilon}|n\rangle\langle n| + |m\rangle\langle m| = 1, \tag{3.110}$$

we have,

$$\sigma_{xy} = \frac{e^2}{\hbar}\frac{1}{2\pi i}\int d^2\mathbf{k}\int d^2\mathbf{r}\left(\frac{\partial u^*_{k_xk_y}}{\partial k_y}\frac{\partial u_{k_xk_y}}{\partial k_x} - \frac{\partial u^*_{k_xk_y}}{\partial k_x}\frac{\partial u_{k_xk_y}}{\partial k_y}\right). \tag{3.111}$$

This can be written as,

$$\sigma_{xy} = \frac{e^2}{\hbar}\frac{1}{2\pi i}\int d^2\mathbf{k}\int d^2\mathbf{r}\left(\nabla_{k_y}u^*_{k_xk_y}\nabla_{k_x}u_{k_xk_y} - \nabla_{k_x}u^*_{k_xk_y}\nabla_{k_y}u_{k_xk_y}\right). \tag{3.112}$$

Let us define here a vector field in the magnetic BZ,

$$\vec{A}(k_x,k_y) = \int d^2\mathbf{r}u^*_{\vec{k}}(\vec{r})\vec{\nabla}ku_{\vec{k}}(\vec{r}),$$

$$=\langle u_{k_x,k_y}|\vec{\nabla}k|u_{k_x,k_y}\rangle, \tag{3.113}$$

where $\vec{\nabla}k$ is vector operator whose component are $\frac{\partial}{\partial k_x}$ and $\frac{\partial}{\partial k_x}$. Using Eq. (3.113) and (3.112) becomes,

$$\sigma_{xy} = \frac{e^2}{\hbar}\frac{1}{2\pi i}\int d^2\mathbf{k}\left(\vec{\nabla}_{\vec{k}} \times \vec{A}(k_x, k_y)\right)_3. \tag{3.114}$$

Here, $()_3$ is the third component of the vector. The integration is over magnetic BZ defined in (3.87).

Let's discuss first gauge transformation. Suppose, $u_{k_xk_y}(x, y)$ is the solution of the Schrodinger equation

$$\left(\frac{\left(\vec{p} + \hbar\vec{k} - \frac{e}{c}\vec{A}\right)^2}{2m} + U(x, y)\right) u_{k_xk_y}(x, y) = \varepsilon u_{k_xk_y}(x, y), \tag{3.115}$$

then the $u_{k_xk_y}(x, y)\exp(if(k_x, k_y))$ also satisfies the Eq.(3.115). Where, $f(k_x, k_y)$ is an arbitrary smoothly varying function of k_x and k_y. This function does not depend upon x and y. This introduces a transformation,

$$u'_{k_xk_y}(x, y) = u_{k_xk_y}(x, y)\exp(if(k_x, k_y)). \tag{3.116}$$

Since this transformation only changes the overall phase of the wave-function, so any physical observable quantity remains invariant under this transformation. The $\hat{\mathbf{A}}(k_x, k_y)$ transform as,

$$\begin{aligned}\hat{\mathbf{A}}'(k_x, k_y) &= \int d^2r u^{*\prime}(k_xk_y)\vec{\nabla}_{\vec{k}}u'_{k_xk_y},\\ &= \hat{\mathbf{A}}(k_x, k_y) + i\nabla_{\vec{k}}f(k_x, k_y)\int d^2r u^*_{k_xk_y}u_{k_xk_y},\\ &= \hat{\mathbf{A}}(k_x, k_y) + i\nabla_{\vec{k}}f(k_x, k_y).\end{aligned} \tag{3.117}$$

We use here, $\int d^2r u^*_{k_xk_y}u_{k_xk_y} = 1$. The expression of conductivity under this transformation becomes,

$$\sigma_{xy} = \frac{e^2}{h}\frac{1}{2\pi i}\int d^2k\left(\vec{\nabla}_{\vec{k}} \times \hat{\mathbf{A}}'(k_x, k_y)\right)_3. \tag{3.118}$$

Using the vector identity ,

$$\vec{\nabla} \times \vec{\nabla}f = 0, \tag{3.119}$$

we have,

$$\sigma_{xy} = \frac{e^2}{h}\frac{1}{2\pi i}\int d^2k\left(\vec{\nabla}_{\vec{k}} \times \hat{\mathbf{A}}(k_x, k_y)\right)_3. \tag{3.120}$$

This shows that σ_{xy} remains invariant under this gauge transformation, if $f(k_x, k_y)$ is determined uniquely and smoothly in the entire magnetic BZ.
Now consider the case where wave-function $u_{k_x k_y}(x, y)$ is zero for some value of $k_x^{(0)}$ and $k_y^{(0)}$ in the magnetic BZ. We divide the magnetic BZ into two pieces H_I and H_{II} such that H_I contains $\left(k_x^{(0)}, k_y^{(0)}\right)$ as shown in fig.(3.3). At the boundary

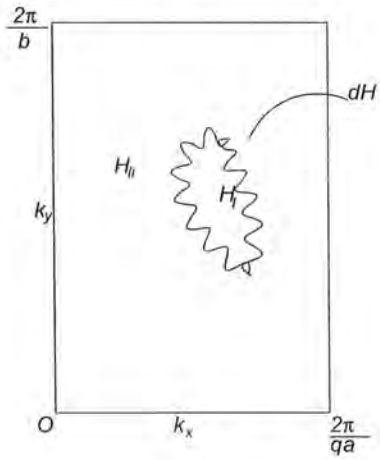

FIGURE 3.3: Schematic diagram of a phase of a wavefunction in the magnetic Brillouine zone.

of H_I and H_{II} we have a phase relation between the state vectors,

$$|u^{II}_{k_x k_y}\rangle = \exp\left(i\chi(k_x, k_y)\right)|u^{I}_{k_x k_y}\rangle, \tag{3.121}$$

where $\chi(k_x, k_y)$ is smoothly varying function of k_x and k_y on the boundary of the H_I and $h_I I$. This implies that,

$$\hat{\mathbf{A}}(k_x, k_y)_{II} = \hat{\mathbf{A}}(k_x, k_y)_I + i\vec{\nabla}_{\vec{k}}\chi(k_x, k_y). \tag{3.122}$$

The expression for conductivity (3.114) becomes,

$$\sigma_{xy} = \frac{e^2}{h}\frac{1}{2\pi i}\int_{H_I} d^2k\left(\vec{\nabla}_{\vec{k}} \times \hat{\mathbf{A}}_I(\vec{k})\right)_3 + \int_{H_{II}} d^2k\left(\vec{\nabla}_{\vec{k}} \times \hat{\mathbf{A}}_{II}(\vec{k})\right)_3. \tag{3.123}$$

By applying Stokes law separately, we obtain,

$$\sigma_{xy} = \frac{e^2}{h}\frac{1}{2\pi i}\int d\vec{k}\cdot\left(\hat{\mathbf{A}}_I - \hat{\mathbf{A}}_{II}\right), \tag{3.124}$$

$$\begin{aligned}\sigma_{xy} =& \frac{e^2}{h}\frac{1}{2\pi i} i \int d\vec{k} \cdot \vec{\nabla}\chi, \\ =& \frac{e^2}{h}\frac{1}{2\pi}(\chi_i - \chi_f).\end{aligned} \tag{3.125}$$

Since, $(\chi_i - \chi_f) = 2\pi n$ for the single valuedness of the state vector at the boundary of the H_I and H_{II}. Thus, we obtain,

$$\sigma_{xy} = \frac{e^2}{h} n. \tag{3.126}$$

The conductivity is quantized in the unit of $\frac{e^2}{h}$. We used here gauge invariance argument to quantize the conductivity.

3.4 2DEG in an arbitrary electric and perpendicular magnetic fields

We appraise here an alternative frame work for understanding the behaviour of the two-dimensional electron gas in a large perpendicular magnetic field and spatially varying electric field. We investigate here electronic and thermal properties of electron gas. The sample geometry is rectangular of length L_x and width L_y along x and y direction respectively. The Hamiltonian in the presence of the magnetic and electric field can be written as,

$$\mathcal{H} = \frac{\Pi_x^2}{2m} + \frac{\Pi_y^2}{2m} + eV(x, y). \tag{3.127}$$

By using raising and lowering operator define in (3.7), we can write Hamiltonian as,

$$\mathcal{H} = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) + eV(x, y). \tag{3.128}$$

We choose here a representation where one of the guiding centre coordinate is diagonal say X. So Y is forced to be indefinite because,

$$[X, Y] = -il_B^2. \tag{3.129}$$

The non-commutativity means that (X, Y) can generate the entire phase space with the cells of size $2\pi l_B^2$. This non-commutativity is the main reason of degeneracy of Landau levels which we discuss later in this section. The commutation

relation between X and Y implies the following matrix element,

$$\langle Y|X\rangle = \frac{1}{\sqrt{L_y}} \exp\left(-i\frac{XY}{l_B^2}\right). \tag{3.130}$$

If the potential is arbitrary, i.e., it depends upon x as well as y coordinate, then it is unhelpful to choose X eigenstate because, $[X, \mathcal{H}] \neq 0$. Let us assume that the potential has only x dependence, i.e., $V(x, y) = U(x)$.

3.4.1 Degeneracy of Landau levels

As electrons are free in Y-direction so we can rightfully insist that

$$\langle Y + L_y|x\rangle = \langle Y|X\rangle. \tag{3.131}$$

This imply that

$$\frac{1}{\sqrt{L_y}} \exp\left(-i\frac{XY}{l_B^2}\right) = \frac{1}{\sqrt{L_y}} \exp\left(-i\frac{X(Y + L_y)}{l_B^2}\right). \tag{3.132}$$

This restricts X to a certain discrete values, i.e.,

$$X_m = \frac{2\pi l_B^2}{L_y} m. \tag{3.133}$$

As the all values of X lies between,

$$0 < X_m < L_x. \tag{3.134}$$

This implies that for some maximum value of $M = \frac{\Phi}{\Phi_0}$ the $X_M \leq L_x$. So each Landau level is hugely degenerate.

3.5 Hamiltonian and energy eigenvalues

Now consider a Hamiltonian in which the potential is only x-dependent. Since under this approximation $[X, \mathcal{H}] = 0$, so energy eigenvalues can be labelled by X. We assume that the potential is smooth enough to approximate linear in any ΔX. So E_X is constant in any interval ΔX and E_X is very large near the edges such that it confines the electrons inside the sample and have any arbitrary form in the

Bulk of the sample. If we expand $U(x)$ we have,

$$U(x) = U(X) - xE_X. \tag{3.135}$$

The Hamiltonian in (3.128) becomes,

$$\mathcal{H} = \frac{\Pi_x^2}{2m} + \frac{\Pi_y^2}{2m} + e\sum_X (U(X) - xE_X). \tag{3.136}$$

Using the value of x in (3.22) and ladder operators define in (3.7) we have,

$$\mathcal{H} = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) + e\sum_X \left[U(X) - \left(X - \frac{c}{eB}\Pi_y\right)\right]. \tag{3.137}$$

By arranging and using the value of Π_y defined in (3.15) we obtain,

$$\mathcal{H} = \sum_X \left[\hbar\omega\left(a^\dagger a + \frac{1}{2}\right) + \frac{ieE_X l_B}{\sqrt{2}}\left(a^\dagger - a\right) + e\left(U_X - XE_X\right)\right]. \tag{3.138}$$

To keep the notation simple, let us define $\beta = \frac{eE_X l_B}{\hbar\omega}$. One can write the above Hamiltonian using this value of β as,

$$\mathcal{H} = \hbar\omega_c \sum_X \left(a^\dagger a + \frac{1}{2} + \frac{i\beta}{\sqrt{2}} - \frac{i\beta}{\sqrt{2}}\right) + e\sum_X \left(U_X - XE_X\right), \tag{3.139}$$

$$= \hbar\omega_c \sum_X \left[\left(a^\dagger + \frac{i\beta}{\sqrt{2}}\right)\left(a - \frac{i\beta}{\sqrt{2}}\right) + \frac{1}{2}\left(1 - \beta^2\right)\right] + e\sum_X \left(U_X - XE_X\right). \tag{3.140}$$

Now let us define two new ladder operators as,

$$A_X^\dagger = a^\dagger + \frac{i\beta}{\sqrt{2}},$$
$$A_X = a - \frac{i\beta}{\sqrt{2}}. \tag{3.141}$$

We can check that the new definition of the ladder operators preserve the usual commutation relation, i.e.,

$$\left[A_X^\dagger, A_X\right] = 1. \tag{3.142}$$

The final form of the Hamiltonian is given by

$$\mathcal{H} = \hbar\omega \sum_X \left[A_X^\dagger A_X + \frac{1}{2}\left(1 - \beta^2\right)\right] + e\sum_X \left(U_X - XE_X\right). \tag{3.143}$$

Now to calculate the ground state wave function we need to consider the following property of ladder operator

$$A_X|0,X\rangle = 0. \tag{3.144}$$

We can see that it is not killed by ordinary lowering operator a. The complex representation of A_X is given below

$$A_X = -i\sqrt{2}l_B\left(\bar{\partial} + \frac{eB}{4\hbar c}z + \frac{\beta}{2l_B}\right). \tag{3.145}$$

The ground state wave function thus,

$$\langle\bar{z},z| - i\sqrt{2}l_B\left(\bar{\partial} + \frac{eB}{4\hbar c}z + \frac{\beta}{2l_B}\right)|0,X\rangle = 0, \tag{3.146}$$

$$\left(\bar{\partial} + \frac{eB}{4\hbar c}z + \frac{\beta}{2l_B}\right)\varphi_0(z,\bar{z}) = 0, \tag{3.147}$$

$$\Rightarrow \qquad \varphi_0(z,\bar{z}) = \frac{1}{\sqrt{2\pi l_B}}\exp\left(-\frac{z\bar{z}}{4l_B^2} - \frac{\beta z}{2l_B}\right). \tag{3.148}$$

The energy eigenvalues are local and given by the equation,

$$\varepsilon_{n,X} = \hbar\omega\left[n + \frac{1}{2}\left(1-\beta^2\right)\right] + e\left(U_X - XE_X\right). \tag{3.149}$$

The position operators of electron are,

$$\begin{aligned} x =& X - \frac{c}{eB}\Pi_y \\ \Rightarrow x =& X + \frac{il_B}{\sqrt{2}}\left(A_X^\dagger - A_X\right) + \beta l_B \end{aligned} \tag{3.150}$$

$$\begin{aligned} y =& Y + \frac{c}{eB}\Pi_x \\ \Rightarrow y =& Y + \frac{l_B}{\sqrt{2}}\left(A_X + A_X^\dagger\right) \end{aligned} \tag{3.151}$$

The average value of x in any Landau Level is,

$$\begin{aligned} \langle x\rangle =& \langle n,X|X + \frac{il_B}{\sqrt{2}}\left(A_X^\dagger - A_X\right) + \beta l_B|n,X\rangle, \\ =& \frac{il_B}{\sqrt{2}}\langle n,X|A_X^\dagger|n,X\rangle + \frac{il_B}{\sqrt{2}}\langle n,X|A_X|n,X\rangle + X + \beta l_B, \\ =& X + \beta l_B. \end{aligned} \tag{3.152}$$

Similarly,

$$\langle y\rangle = Y. \tag{3.153}$$

This shows that in large B limit, $\beta l_B \to 0$. Hence,

$$\langle x \rangle = X, \qquad \langle y \rangle = Y. \tag{3.154}$$

Thus the electrons are localised around the guiding centre. We can understand the above in the following way. First, consider there is no electric field which is the condition of an ideal $2D$ electron gas. The electrons are hugely degenerate and fill up the states upto the Fermi energy and X takes one of the maximum value say X_M. Now we apply the potential which is only x-dependent. Since $\dot{X} = 0$, so X does not change. However, there is a broadening of LLs. This broadening depends upon the value of the internal electric field. Let us now calculate the current flowing through the sample.

3.6 Current and Conductivity

The current flowing in any direction can be calculated by using Heisenberg equation of motion,

$$\begin{aligned} i\hbar\dot{x} =& [x, H] \\ =& \left[X + \frac{il_B}{\sqrt{2}}\left(A_X^\dagger - A_X\right) + \beta l_B, \hbar\omega \sum_X \left[A_X^\dagger A_X + \frac{1}{2}\left(1-\beta^2\right)\right] + e\sum_X \left(U_X - XE_X\right)\right], \\ =& \frac{il_B\hbar\omega}{\sqrt{2}}\left(A_X + A_X^\dagger\right). \end{aligned} \tag{3.155}$$

Hence the current operator in x-direction is,

$$I_x = \frac{el_B\omega}{L_x}\left(A_X + A_X^\dagger\right). \tag{3.156}$$

In the similar way we can find the current operator in the y-direction which is

$$I_y = -\frac{e}{L_y}\left[c\frac{E_X}{B} + i\omega\frac{1}{\sqrt{2}}\left(A_X - A_X^\dagger\right)\right] \tag{3.157}$$

The average value of the current operator in x-direction in any Generalised Landau Level(GLL) is,

$$\langle I_x \rangle = \langle n, X | \frac{el_B\omega}{L_x}\left(A_X + A_X^\dagger\right) | n, X \rangle = 0. \tag{3.158}$$

The average value of the current operator in any interval ΔX is,

$$I_y^{\Delta X} = -\frac{e}{L_y} c \frac{E_X}{B}. \tag{3.159}$$

The total current can be obtained by adding the current in all strips, i.e.,

$$\begin{aligned} I_y &= \sum_X I_y^{\Delta X}, \\ &= -\frac{e}{L_y} \sum_X \frac{\Delta X L_y}{2\pi l_B^2} \times c \frac{E_X}{B}, \\ &= -\frac{e^2}{h} \int dX E_X = \frac{e^2}{h} V. \end{aligned} \tag{3.160}$$

One reads the Hall conductance,

$$\sigma_{xy} = \frac{e^2}{h}. \tag{3.161}$$

Since each filled Landau Level contribute same amount to the conductivity. Hence,

$$\sigma_{xy} = n \frac{e^2}{h}. \tag{3.162}$$

Here is point to be noted: as the current flows in any interval ΔX is proportional to the value of E_X so the current will flow wherever electric field is present even in the bulk. Since there is a strong electric field near the edges so more current flows near the edges of the sample.

The importance of this calculation lies in the fact that we use arbitrary piecewise linear potential rather than ideal 2-D electron gas. Translational symmetry is broken, we do not have a frame of reference where electric field made to vanish. Thus the electrical conductance is quantized.

3.7 Heat current

Now let us assume that the system is attached to a heat bath with a temperature gradient along y-direction, i.e., T_+ on the upper end and T_- on the lower end. The temperature gradient is given by,

$$\nabla_y T = \frac{T_+ - T_-}{L_y} = \frac{\Delta T}{L_y}. \tag{3.163}$$

Here we are going to focus our attention to the heat current in the ballistic transport regime, i.e., the pure semi-conductor and low temperature, low enough that the mean free path is greater than the sample size and linear response theory works. We predict here when the Fermi energy lies in the gap between two GLL's, the thermal conductance is perfectly quantized. The charges moves ballistic-ally from upper end to the lower end equilibrated fermi distribution $f(\mu_+, T_+)$ and the charges moves from lower end to upper end are equilibrated with the fermi function $f(\mu_-, T_-)$. The resulting heat current can be calculated by using the Landauer formula (2.181). The heat current is,

$$\langle I_Q \rangle = \langle (\varepsilon - \mu)\, \dot{Y} \rangle. \tag{3.164}$$

Where ε is energy per particle and $\dot{Y}$ is velocity of electron in the y-direction can be calculated by the Heisenberg EOM as,

$$i\hbar \dot{Y} = [Y, \mathcal{H}(\mathbf{R})], \tag{3.165}$$

where the Hamiltonian does not depend explicitly on $\mathbf{R}$ but through potential. Hence,

$$i\hbar \dot{Y} = [Y, X] \frac{\partial \mathcal{H}}{\partial X} = i l_B^2 \frac{\partial \mathcal{H}}{\partial X}. \tag{3.166}$$

Hence,

$$\dot{Y} = \frac{l_B^2}{\hbar} \frac{\partial \mathcal{H}}{\partial X}. \tag{3.167}$$

The average value of $\dot{Y}$ in any GLL can be calculated as,

$$\langle \dot{Y} \rangle = \langle n, X | \dot{Y} | n, X \rangle = \frac{l_B^2}{\hbar} \frac{\partial \varepsilon_{n,X}}{\partial X}. \tag{3.168}$$

The average value of the heat current by using the Landauer formula (2.181) can be written as,

$$I_Q = \frac{1}{L_y} \frac{L_y}{2\pi l_B^2} \sum_n \int_0^{X_M} dX\, (\varepsilon - \mu) \times \frac{l_B^2}{\hbar} \frac{\partial \varepsilon_{n,X}}{\partial X} \left[f\left(\mu_+(X), T_+(X)\right) - f\left(\mu_-(X), T_-(X)\right) \right],$$

where $T_n(\varepsilon) = 1$ for the perfect transmission. Thus,

$$I_Q = \frac{1}{2\pi\hbar} \sum_n \int_{\varepsilon_0(n)}^{\varepsilon_1(n)} d\varepsilon (\varepsilon - \mu) \left[f\left(\mu_+(X), T_+(X)\right) - f\left(\mu_-(X), T_-(X)\right) \right]. \tag{3.169}$$

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Here, $\varepsilon_0(n) = \varepsilon_{n,0}$, and $\varepsilon_1(n) = \varepsilon_{n,X_M}$. We define,

$$\mu = \frac{\mu_+ + \mu_-}{2}, \qquad T = \frac{T_+ + T_-}{2}. \tag{3.170}$$

In order to compute linear response, we expand the Fermi function around the averages. Thus we get,

$$f(\mu_+, T_+) - f(\mu_-, T_-) = \left(\Delta\mu - \frac{\varepsilon - \mu}{T}\Delta T\right)\frac{\partial f}{\partial x}, \tag{3.171}$$

where $x = \frac{\varepsilon - \mu}{k_B T}$. Thus the expression for the current in (3.169) becomes,

$$I_Q = \frac{k_B T}{h}\sum_n \int_{x_0}^{x_1} dx \left(\Delta\mu x \frac{\partial f}{\partial x} - k_B \Delta T x^2 \frac{\partial f}{\partial x}\right). \tag{3.172}$$

Where,

$$x_1 = \frac{\varepsilon_1(n) - \mu}{k_B T}, \qquad x_2 = \frac{\varepsilon_2(n) - \mu}{k_B T}. \tag{3.173}$$

The derivative of fermi function is,

$$\frac{\partial f}{\partial x} = \frac{-1}{4cosh^2\frac{x}{2}}. \tag{3.174}$$

Thus the equation (3.172) becomes,

$$I_Q = \frac{k_B T}{h}\left[\Delta\mu \sum_n A_1(n) + k_B \Delta T \sum_n A_2(n)\right]. \tag{3.175}$$

Here we define,

$$A_\nu(n) = \int_{x_0}^{x_1} dx \frac{x^\nu}{4cosh^2\frac{x}{2}}. \tag{3.176}$$

The integral defined in (3.176) can be evaluated for $\nu = 1, 2$. At the low temperature limit, $x_0 \to -\infty$, and $x_1 \to \infty$. Hence the integral in (3.176) becomes,

$$\begin{aligned} A_1(n) &= \int_{-\infty}^{+\infty} dx \frac{x}{4\cosh^2\frac{x}{2}} = 0, \\ A_2(n) &= \int_{-\infty}^{+\infty} dx \frac{x^2}{4\cosh^2\frac{x}{2}} = \frac{\pi^2}{3}. \end{aligned} \tag{3.177}$$

The heat current in (3.175) is,

$$I_Q = \sum_n \frac{\pi k_B^2 T}{3h} \times \Delta T. \tag{3.178}$$

Thermal conductance can be read as,

$$G_Q = \frac{\pi k_B^2 T}{3h} M. \tag{3.179}$$

Hence we arrive our result that the thermal conductivity is quantized.

Chapter 4

Electronic and thermal properties of graphene

We review here the basic aspects of the electrons in graphene subjected to a strong perpendicular magnetic field. One of its most interesting features is the relativistic quantum Hall effect. The RQHE may be understood in terms of Landau quantization for massless Dirac fermions, which is also the theoretical basis for the understanding of more involved phenomena due to electron interaction. We present the role of mass confinement in integer filling of Landau levels. Furthermore, we discuss briefly the mesoscopic transport in a graphene sample.

4.0.1 Graphene structure

Graphene is a two dimensional layer of carbon atoms ordered into a honeycomb lattice as shown in figure (4.1), theoretically was described 60 years ago. Since, that time the band structure calculation of carbon has been done many times. These calculations have been also used to describe the various properties of carbon. The theoretical discussion of 2-D crystal is started in $1940's$, when Landau and Peirls argued that 2-D crystal does not exist. Therefore, no one tried seriously to create a two dimensional sheet of atoms. However, in 2004, K.Novoselov et al.3.45 got hold of a two-dimensional sheet of carbon atoms. This elusive two-dimensional form of carbon atoms is called Graphene. It is one of the most interesting and theoretically studied allotropes of carbon.

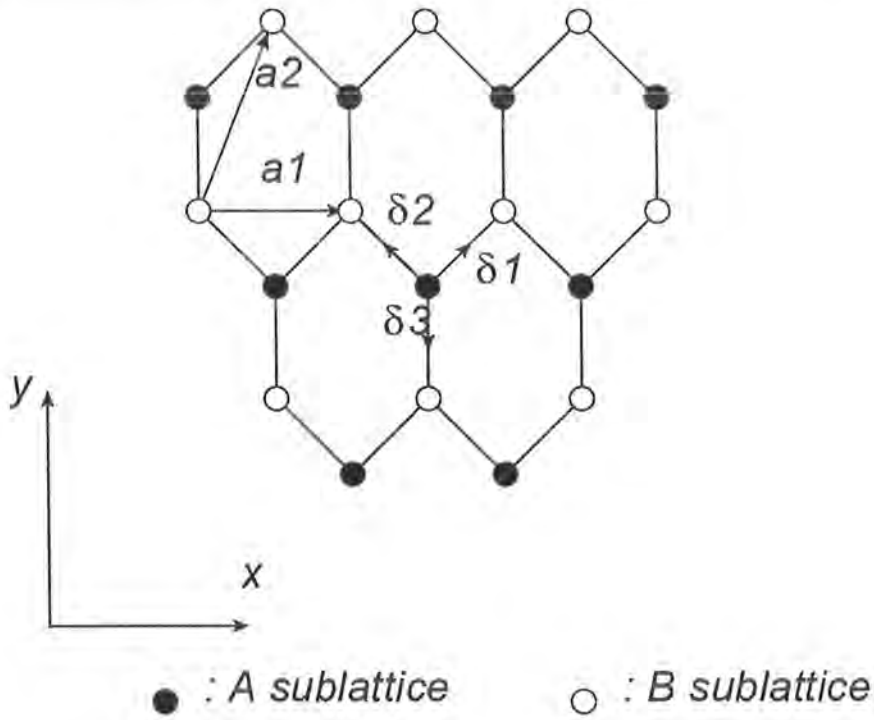

FIGURE 4.1: Honeycomb lattice. The vectors δ_1, δ_2, and δ_3 connect nn carbon atoms, separated by a distance $a = 0.142$ nm. The vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ are the basis vectors of the triangular Bravais lattice.

The electronic structure of graphene has two atoms per unit cell which results in two conical points per Brillouin zone with the band crossing, K and K'. Near these crossing points the electron energy is linearly dependent on the wave vector. Actually, this behaviour follows from symmetry considerations and thus is robust with respect to long-range hopping processes.

What makes graphene so attractive for research is that the spectrum nearly resembles the spectrum of the massless Dirac fermions. The Dirac equation deals with relativistic quantum particles with spin 1/2 such as electron and proton. The essential feature of the Dirac equation is that the states at positive and negative energy are linked. They can be described by different components of the same spinor wave function. For massless Dirac fermions the energy gap between electron energy and maximal positron energy becomes zero and linear dispersion law holds.

The fact that charge particles in graphene are described by the Dirac-like Hamiltonian rather than the usual Schrodinger equation. This can be visualised

as a result of graphene's crystal structure, which consists of two equivalent two sub-lattices A and B. Quantum mechanical hopping between two sub-lattices leads to the formation of two energy bands near the edges of Brillouin zone resulting in the conical energy spectrum. As a result, the charge particles in graphene are described by the Dirac Hamiltonian,

$$\mathcal{H}_{\mathcal{D}} = \hbar v_F(\vec{\sigma} \cdot \vec{p}). \tag{4.1}$$

This is derived in appendix(A). Here, $v_F \approx c/300$, plays the role of speed of light. Due to the linear spectrum one can expect that the properties of graphene behaves differently from usual metals where the dispersion relation is parabolic.

4.1 Chirality in graphene

Charility in the graphene is the same as the the chirality in the ultra relativistic Dirac equation. $\vec{\sigma} \cdot \hat{p}$ is known as chirality operator. There are two eigenvalues corresponding to the chirality operator, i.e.,

$$\vec{\sigma} \cdot \hat{p}\Psi_{\pm} = \pm 1\Psi_{\pm}, \tag{4.2}$$

where $+1$ corresponds to pseudospin parallel to momentum and -1 corresponds to pseudospin anti-parallel to momentum. Another interpretation is that for a given $\vec{p}$ there are two chiral states, a positive energy state and a negative energy state. One interesting effect of chirality is Klein tunneling. We will better understand this concept in the next section.

4.1.1 Klein tunnelling

The Dirac Hamiltonian for graphene is,

$$H_D = \vec{\sigma} \cdot \vec{p} = \begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix}. \tag{4.3}$$

The solution of the eigenvalue equation is a plane wave can be written as,

$$\Psi = \begin{pmatrix} a \\ b \end{pmatrix} \exp(ik_x x + ik_y y). \tag{4.4}$$

The eigenvalue is,

$$\epsilon = \pm v_F \hbar |\vec{k}|. \tag{4.5}$$

To find the values of a and b, we use the following equations,

$$(H_D - \epsilon)\Psi = 0, \tag{4.6}$$

$$a^2 + b^2 = 1. \tag{4.7}$$

Equation (4.6) implies that

$$\begin{pmatrix} -\epsilon & v_F(p_x - ip_y) \\ v_F(p_x + ip_y) & -\epsilon \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} \exp(ik_x x + ik_y y) = 0. \tag{4.8}$$

This gives two coupled equations,

$$-\epsilon a + v_F(k_x - ik_y)b = 0, \tag{4.9}$$

$$v_F(k_x + ik_y)a - \epsilon b = 0. \tag{4.10}$$

By solving these two coupled equations, we have,

$$a = \pm \frac{k_x - ik_y}{|\vec{k}|} b, \tag{4.11}$$

$$b = \pm \frac{k_x - ik_y}{|\vec{k}|} a. \tag{4.12}$$

If we define for some values of k_x and k_y,

$$\exp(\pm i\theta) = \frac{k_x \pm ik_y}{|\vec{k}|}. \tag{4.13}$$

We can write the above equations as,

$$a = \exp(-i\theta)b, \qquad b = \exp(i\theta)a. \tag{4.14}$$

This shows that $|a| = |b|$. Hence,

$$\Psi_\pm = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm \exp(-i\theta) \\ 1 \end{pmatrix} \exp(ik_x x + ik_y y). \tag{4.15}$$

Now consider the Dirac Hamiltonian for graphene in the presence of a potential $V(x)$,

$$\mathcal{H} = v_F \vec{\sigma} \cdot \vec{p} + V(x) I, \tag{4.16}$$

where $V(x)$ varies only in the $x-$direction, I is identity operator. Since the Hamiltonian is translationally invariant in the y-direction, p_y is conserved. Let us choose $V(x)$ to be a step function,

$$V(x) = \begin{cases} -\frac{V_0}{2} & x < 0 \\ \frac{V_0}{2} & x > 0, \end{cases} \tag{4.17}$$

so that the wave function on the both sides of the barriers are same as we found previously with energy,

$$E = V(x) \pm v_F \hbar |\vec{k}|. \tag{4.18}$$

Now let us consider a situation for which an incoming wave on the left side of the barrier have $E = 0$, i.e., $\pm\hbar v_F|\vec{k}| = \frac{V_0}{2}$. This implies that we have to choose minus sign in equation (4.15) and (4.18), to satisfy this condition. Similarly, right side of the barrier we have to choose negative sign. Since minus sign corresponds to holes, if p_x is momentum in left side of the barrier then it should be $-p_x$ in the right side of the barrier.

Now consider a wave incident on the junction from the left side, then for $x < 0$, we can write,

$$\Psi_{x<0} = \frac{1}{\sqrt{2}} \begin{pmatrix} -\exp(-i\theta) \\ 1 \end{pmatrix} \exp(ik_x x + ik_y y) + \frac{r}{\sqrt{2}} \begin{pmatrix} -\exp(i\theta) \\ 1 \end{pmatrix} \exp(-ik_x x + ik_y y). \tag{4.19}$$

Here r is amplitude of reflected wave from the barrier. For reflected wave, $k_x \to -k_x$, and $\frac{-k_x + ik_y}{|\vec{k}|} = \exp(i\theta)$. The wave function on the right side of the junction can be written as,

$$\Psi_{x>0} = \frac{t}{\sqrt{2}} \begin{pmatrix} \exp(i\theta) \\ 1 \end{pmatrix} \exp(-ik_x x + ik_y y), \tag{4.20}$$

where t is transmitted amplitude of the wave. The continuity of the wave function at $x = 0$ gives,

$$\exp(-i\theta) - r\exp(i\theta) = t\exp(i\theta), \tag{4.21}$$

$$1 + r = t. \tag{4.22}$$

One can solve these equations for the values of t and r,

$$t = \frac{1 + \exp(2i\theta)}{2}, \qquad r = \frac{\exp(-2i\theta) - 1}{2}. \tag{4.23}$$

Let, $T = |t|^2$ is transmission probability and, $R = |r|^2$ is reflection probability, then,

$$T = \cos^2\theta, \qquad R = \sin^2\theta. \tag{4.24}$$

If a particle is incident normally on the barrier, $p_y = 0$, equation (4.13) becomes,

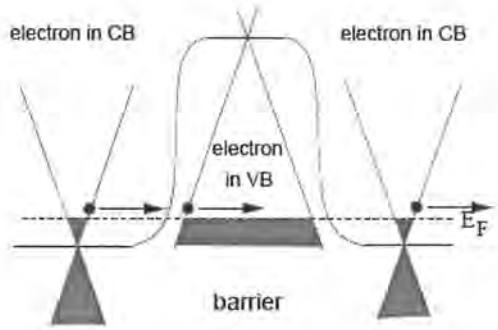

FIGURE 4.2: klein tunneling through a potential barrier. An incident electron in the conduction band above the Fermi energy, which is at the Dirac point before the barrier, transverses the barrier as en electron above the Fermi energy in the valence band. The valence band is partially emptied because the Dirac point has shifted to a higher energy corresponding to the barrier height.

$\exp(i\theta) = 1$. This implies that $\theta = 2m\pi$, where m is an integer. For these values of θ, $T = 1$ and, $R = 0$. Note that: the transmission probability is independent of V_0. Hence, an electric potential cannot confine the Dirac particles. This effect may be understood in the following manner: consider an incident electron in the region with $\frac{-V_0}{2}$ the energy of which is slightly above the Fermi energy. In the potential barrier, the Dirac point is shifted to a higher energy that corresponds to the barrier height and the Fermi energy lies now in the valence band, where the electron may still find a quantum state (with the same wave-vector direction and the same velocity v) instead of moving as an electron in the conduction band, it thus simply moves in the same direction as an electron in the valence band (4.2). To overcome this problem we use mass confinement which will be discussed in the next section.

4.2 Mass confinement

As we discussed in the previous section an electrostatic potential cannot confine the Dirac electrons, this issue is resolved by using a mass term $M\sigma_z$ which is added

in the Dirac Hamiltonian. Hence,

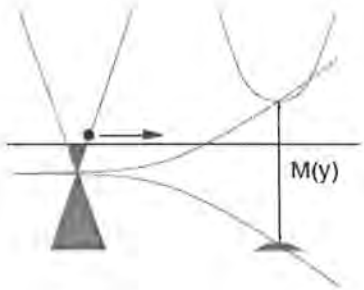

FIGURE 4.3: A gap opens when a particle approaches to the edge, which is forbidden region.

$$\mathcal{H}_D^m = v_F\vec{\sigma}\cdot\vec{p} + M\sigma_z = \begin{pmatrix} M & v_F(p_x - ip_y) \\ v_F(p_x + ip_y) & -M \end{pmatrix}. \tag{4.25}$$

The wave function correspond to this Hamiltonian is given in equation (4.15), and energy spectrum is,

$$\varepsilon_\pm(\vec{k}) = \pm\sqrt{v_F^2\hbar^2|\vec{k}|^2 + M^2}. \tag{4.26}$$

which is gapped at zero momentum. Note that when an electron approaches to the edge where, $M \neq 0$ a gap opens as shown in fig.(4.3). An electron slightly above the Dirac point may then only propagate in the region with $M = 0$, whereas at the edge its energy lies in the gap which is a forbidden region and, the electron is thus confined.

4.3 Dirac fermions in magnetic field

We now consider the problem of a uniform magnetic field **B** applied perpendicular to the graphene sample. We use Landau gauge: $\mathbf{A} = B(-y, 0)$. Note that magnetic field introduces a new scale length in the problem,

$$l_B = \sqrt{\frac{\hbar c}{eB}}, \tag{4.27}$$

which is the magnetic length defined earlier. The only other scale is fermi velocity. Dimensional analysis shows that only quantity, $\hbar v_F/l_B$, has the dimensions of

energy which allows us to define cyclotron frequency,

$$\omega_c = \frac{\sqrt{2}v_F}{l_B}. \tag{4.28}$$

Equations defined in (4.28) and (4.27) show that the cyclotron energy varies as $\sqrt{B}$ rather than in non-relativistic case where cyclotron energy varies linear in B. This implies that energy scale associated with the Dirac fermions is different from the scale associated with the ideal 2D electron gas. Moreover, if the magnetic field is of the order of, $B \sim 10T$, the cyclotron energy of the ideal 2D electron gas is of the order of $10K$. Whereas, the cyclotron energy of Dirac fermion is of the order of $.83eV$, that is, two order of magnitude greater than the ideal 2D electron gas. This has a very strong implication to observe Quantum Hall Effect at room temperature. Further, the Zeemann energy at strong magnetic field relatively small $\approx 6.1 \times 10^{-4}eV$, can be ignored in a high magnetic field limit.
We now consider Dirac equation (4.1) in more detail,

$$\mathcal{H}_{\mathcal{D}} = \hbar v_F(\vec{\sigma} \cdot \vec{p}) = \hbar v_F \left(\sigma_x p_x + \sigma_y p_y\right). \tag{4.29}$$

Here, σ_x and σ_y are Pauli matrices. The Dirac Hamiltonian (4.29) in terms of matrix form is,

$$\mathcal{H}_{\mathcal{D}} = v_F \begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix}. \tag{4.30}$$

Using the minimal coupling to encount the effect of magnetic field the above Hamiltonian becomes,

$$\mathcal{H}_{\mathcal{D}} = v_F \begin{pmatrix} 0 & (p_x + \frac{eB}{c}y) - ip_y \\ (p_x + \frac{eB}{c}y) + ip_y & 0 \end{pmatrix}. \tag{4.31}$$

In the Landau gauge the generic solution of the Dirac equation is of the form,

$$\Psi(x, y) = \exp\left(iky\right) \begin{pmatrix} u \\ v \end{pmatrix}, \tag{4.32}$$

and the Dirac equation then reads,

$$v_F \begin{pmatrix} 0 & (\hbar k + \frac{eB}{c}y) + \nabla_y \\ (\hbar k + \frac{eB}{c}y) - \nabla_y & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = E \begin{pmatrix} u \\ v \end{pmatrix}. \tag{4.33}$$

Using the definition of, $y_0 = -kl_B^2$, the above equation (4.33) becomes,

$$\hbar\frac{\sqrt{2}v_F}{l_B}\begin{pmatrix} 0 & \frac{1}{\sqrt{2}}(\partial_\xi + \xi) \\ \frac{1}{\sqrt{2}}(-\partial_\xi + \xi) & 0 \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} = E\begin{pmatrix} u \\ v \end{pmatrix}. \tag{4.34}$$

Here we define,

$$\xi = \frac{y - y_0}{l_B}. \tag{4.35}$$

And the usual harmonic oscillator operator are defined,

$$\begin{aligned} O &= \frac{1}{\sqrt{2}}(\partial_\xi + \xi), \\ O^\dagger &= \frac{1}{\sqrt{2}}(-\partial_\xi + \xi), \end{aligned} \tag{4.36}$$

The equation (4.34) becomes,

$$\hbar\omega_c\begin{pmatrix} 0 & O \\ O^\dagger & 0 \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} = E\begin{pmatrix} u \\ v \end{pmatrix}. \tag{4.37}$$

We can easily verify that the definition of raising and lowering operators in (4.36) preserve the commutation relation $[O, O^\dagger] = 1$. $N = O^\dagger O$, is number operator. The equation (4.37) can be written in the form of coupled spinors as,

$$Ov = \frac{E_n}{\hbar\omega_c}u, \tag{4.38}$$

$$O^\dagger u = \frac{E_n}{\hbar\omega_c}v. \tag{4.39}$$

One can decouple the above equations,

$$O^\dagger O v_n = \left(\frac{E_n}{\hbar\omega_c}\right)^2 v_n. \tag{4.40}$$

This shows that $v_n \propto |n\rangle$ is an eigenstate of number operator. Thus the energy can be written as,

$$E_n = \pm\hbar\omega_c\sqrt{N} = \pm\hbar\frac{v_F}{l_B}\sqrt{2n}. \tag{4.41}$$

This shows that the energy varies as $\sqrt{B}$ rather than the usual ideal electron gas where energy varies linearly with B. We can see that the energy spectrum has $\pm$ signs, + for the conduction band and - sign for valence band. We need to introduce

another index λ. The energy is now labelled by n and λ, i.e.,

$$E_{n,\lambda} = \lambda\hbar\frac{v_F}{l_B}\sqrt{2n}. \tag{4.42}$$

Another notable difference with respect to non-relativistic Landau levels in metals with parabolic bands is the presence of zero energy Landau Level with $n = 0$. This level need to treat separately, and indeed the solution of eigenvalue equation yields an eigenvector,

$$\psi_{v,n} = \begin{pmatrix} 0 \\ |n=0\rangle \end{pmatrix}, \tag{4.43}$$

with single non-vanishing component. As a result zero energy states at K points are restricted to B sub lattice, where those, at the K' have a non-vanishing weight only on A sub lattice. The eigenstate with $n \neq 0$ is,

$$\psi_{n\neq 0,\lambda} = \begin{pmatrix} |n-1\rangle \\ \lambda|n\rangle \end{pmatrix}. \tag{4.44}$$

4.4 Mesoscopic transport in graphene

We describe here the transport properties of graphene in the mesoscopic regime. In this section, we discuss the Landauer formula for graphene using a model of rectangular wave guide which was discussed in chapter 2. Further, we will use this formulae to analyze the transport co-efficient problem into a one dimensional transmission problem.

A common mesoscopic system does not resemble with the wave guide. However, the physics of quantum transport for graphene is same as an infinite rectangular wave guide. We start with an ideal rectangular waveguide for graphene infinitely long in the x-direction. The Dirac electrons are confined in the y-direction. Since the Dirac particles cannot be confined by even an infinite potential, we assume here that the particle becomes infinite massive as it enters the walls. As the electrons move towards the walls they repelled towards $M = 0$ region so that they cannot tunnel through. We assume an infinite mass well at $y = \pm\frac{a}{2}$,

$$M(y) = \begin{cases} 0 & \frac{-a}{2} < y < \frac{a}{2} \\ \infty & \text{otherwise.} \end{cases}$$

The Dirac Hamiltonian in the presence of this mass term is,

$$H_D^m = v_F\vec{\sigma}\cdot\vec{p} + M(y)\sigma_z = \begin{pmatrix} M(y) & v_F(p_x - ip_y) \\ v_F(p_x + ip_y) & -M(y) \end{pmatrix} \tag{4.45}$$

In order to obtain the eigenvalues and eigenfunction of this Hamiltonian, we need to solve the eigenvalue equation

$$H_D^m\psi(x,y) = \epsilon\psi(x,y), \tag{4.46}$$

where $\psi(x,y)$ is two spinors,

$$\psi(x,y) = \begin{pmatrix} u(x,y) \\ v(x,y) \end{pmatrix}. \tag{4.47}$$

Using this form of wavefunction, one can write the eigenvalue equation as,

$$\begin{pmatrix} M(y) & v_F(p_x - ip_y) \\ v_F(p_x + ip_y) & -M(y) \end{pmatrix}\begin{pmatrix} u(x,y) \\ v(x,y) \end{pmatrix} = \epsilon\begin{pmatrix} u(x,y) \\ v(x,y) \end{pmatrix}, \tag{4.48}$$

hence,

$$M(y)u(x,y) + v_F(p_x - ip_y)v(x,y) = \epsilon u(x,y), \tag{4.49}$$
$$v_F(p_x + ip_y)u(x,y) - M(y)v(x,y) = \epsilon v(x,y). \tag{4.50}$$

After rearranging these coupled equations we have,

$$v_F(p_x - ip_y)v(x,y) = (\epsilon - M(y))\,u(x,y), \tag{4.51}$$
$$v_F(p_x + ip_y)u(x,y) = (\epsilon + M(y))\,v(x,y). \tag{4.52}$$

By applying $v_F(p_x - ip_y)$ on the both sides of the equation(4.50) we obtain,

$$\begin{aligned} &v_F(p_x - ip_y)(p_x + ip_y)u(x,y) = v_F^2(\epsilon + M(y))(p_x - ip_y)v(x,y), \\ &v_F^2(p_x^2 + p_y^2)u(x,y) = v_F^2\left(\epsilon^2 - M^2(y)\right)u(x,y), \\ &\left[p_x^2 + p_y^2 + \frac{M^2(y)}{v_F^2}\right]u(x,y) = \frac{\epsilon^2}{v_F^2}v(x,y). \end{aligned}$$

We can solve this equation by applying the separation of variables technique. By writing $u(x,y) = \chi(x)\phi(y)$, we can decompose the last equation into two one

dimension equations as,

$$p_x^2\chi(x) = \alpha_x\chi(x), \tag{4.53}$$

$$\left[p_y^2 + \frac{M^2(y)}{v_F^2}\right]\phi(y) = \alpha_y\phi(y). \tag{4.54}$$

Here,

$$\frac{\epsilon^2}{v_F^2} = \alpha_x + \alpha_y. \tag{4.55}$$

The solution of equation (4.53) is,

$$\chi(x) = \exp(ik_x x), \qquad \alpha_x = \hbar^2 k_x^2, \tag{4.56}$$

and the solution of the equation (4.54) is,

$$\phi(y) = A\sin k_y y + B\cos k_y y, \tag{4.57}$$

where A and B are arbitrary complex numbers. Since the electrons are are perfectly confined in the transverse direction, the wave function must vanish at $y = \pm\frac{a}{2}$, this condition restricts k_y to certain specific values,

$$k_n = \frac{n\pi}{a}. \tag{4.58}$$

Thus, transverse wave-function and α_y can be written as,

$$\phi_n(y) = A\sin k_n(y - \frac{a}{2}), \qquad \alpha_y = \frac{\hbar^2\pi^2 n^2}{a^2}. \tag{4.59}$$

Hence,

$$u_n(k_x) = A\exp(ik_x x)\sin k_n(y - \frac{a}{2}), \tag{4.60}$$

and energy is given by the equation

$$\epsilon_{n,\lambda}(k_x) = \lambda\sqrt{v_F^2\hbar^2 k_x^2 + \frac{\hbar^2 v_F^2\pi^2}{a^2}n^2}. \tag{4.61}$$

Where $\lambda = +$ for the conduction band and $\lambda = -$ for the valence band. Now let us look for the other spinor $v(x, y)$. From equation (4.52),

$$\begin{aligned} v_n(k_x) &= \frac{v_F}{\epsilon_{n,\lambda}(k_x) + M(y)} (p_x + ip_y)\, u_n(k_x), \\ &= \frac{Av_F \exp(ik_x x)}{\epsilon_{n,\lambda}(k_x) + M(y)} \left(\hbar k_x \sin k_n(y - \frac{a}{2}) + \hbar \frac{d}{dy} \sin k_n(y - \frac{a}{2}) \right), \\ &= \frac{A\hbar k_x v_F \exp(ik_x x)}{\epsilon_{n,\lambda}(k_x) + M(y)} \left(\sin k_n(y - \frac{a}{2}) + \frac{n\pi}{ak_x} \cos k_y^n(y - \frac{a}{2} \right). \end{aligned}$$

Hence, the wave-function becomes,

$$\psi_{n,\lambda}(k_x) = A \exp(ik_x x) \begin{pmatrix} \sin k_n(y - \frac{a}{2}) \\ \frac{\hbar v_F}{\epsilon_{n,\lambda}(k_x)} \left(k_x \sin k_n(y - \frac{a}{2}) + \frac{n\pi}{a} \cos k_n(y - \frac{a}{2}) \right) \end{pmatrix}. \quad (4.62)$$

We put $M(y) = 0$ here, for the region inside the sample. We can easily verify that the particle current along the y-direction is zero by computing j_y,

$$j_y = e\langle \hat{v}_y \rangle \quad (4.63)$$

where $\hat{v}_y$ is velocity operator of the electrons in the y-direction. We can find it by using Heisenberg EOM as follows,

$$i\hbar\dot{y} = [y, H_D] = [y, \sigma_x p_x + \sigma_y p_y] = i\hbar\sigma_y, \quad (4.64)$$

hence,

$$\hat{v}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \quad (4.65)$$

Now,

$$\langle |j_y| \rangle = ei|A|^2 \begin{pmatrix} \sin k_n(y - \frac{a}{2}) & \frac{\hbar v_F}{\epsilon_{n,\lambda}(k_x)} \left(k_x \sin k_n(y - \frac{a}{2}) + \frac{n\pi}{a} \cos k_y^n(y - \frac{a}{2}) \right) \end{pmatrix} \times \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$
$$\begin{pmatrix} \sin k_n(y - \frac{a}{2}) \\ \frac{\hbar v_F}{\epsilon_{n,\lambda}(k_x)} \left(k_x \sin k_n(y - \frac{a}{2}) + \frac{n\pi}{a} \cos k_n(y - \frac{a}{2}) \right) \end{pmatrix},$$

by performing this simple matrix multiplication we obtain the result $j_y = 0$. This shows that electrons are perfectly confined in the transverse direction and free in the longitudinal direction.

Now consider the walls of the waveguide varies, and come closer at $x = 0$ forming

a constriction in the middle, just as we discussed in non-relativistic case but this time we are considering the infinite mass rather than the potential. Now the mass term is,

$$M(a(x), y) = \begin{cases} 0 & \frac{-a(x)}{2} < y < \frac{a(x)}{2} \\ \infty & otherwise. \end{cases} \tag{4.66}$$

Since this mass term does not allow the separation of variables and the solutions of the Dirac equation found previously do not apply in this case. Under the adiabatic conditions discussed in chapter 2, the walls become locally flat and parallel, and the wave function can be approximated by those found previously by replacing, $a \to a(x)$ and energy is,

$$\epsilon_{n,\lambda}(k_x) = \lambda\sqrt{v_F^2\hbar^2k_x^2 + \frac{\hbar^2 v_F^2\pi^2}{a(x)^2}n^2}. \tag{4.67}$$

In spite of the similarity with the non-relativistic case the effective channel dependent potential energies are,

$$\alpha_y(x) = \frac{\hbar^2 v_F^2\pi^2}{a(x)^2}n^2. \tag{4.68}$$

4.5 Quantum transport in graphene

Let us connect the wave-guide with two reservoirs which are at chemical potentials μ_L and μ_R where μ_L is the chemical potential of the left reservoir and μ_R is the chemical potential of the lower reservoir as shown in fig (2.3). These reservoirs inject electrons into the wave-guide. The net current flowing along the x-direction which can be calculated in a similar way as we did for the non relativistic case, by using equation (2.166) which reads as,

$$I_e = \frac{g_s e}{h}\sum_n \int_0^\infty d\epsilon T_n(\epsilon)\left[f(\epsilon-\mu_L) - f_R(\epsilon-\mu_R)\right]. \tag{4.69}$$

Here, g_s is the factor due to the four fold degeneracy of each level, two-fold due to the spin and two-fold due the valley degeneracy and $T_n(\epsilon)$ is energy and channel dependent transmission coefficient. The distribution function $f(\epsilon-\mu)$ is also different from the usual fermion distribution function because the energy spectrum in the relativistic case is linear in k. If the two reservoirs are at different temperatures, i.e., T_L is temperature of the left reservoir and T_R is the temperature of the

right reservoir then the Landauer formula (4.69) becomes,

$$I_e = \frac{g_s e}{h} \sum_n \int_0^\infty d\varepsilon T_n(\varepsilon) \left[f(\varepsilon - \mu_L, T_L) - f(\varepsilon - \mu_R, T_R) \right]. \tag{4.70}$$

Suppose that the waveguide is symmetrically biased, i.e.,

$$T_L = T + \frac{\Delta T}{2}, \qquad T_R = T - \frac{\Delta T}{2}, \tag{4.71}$$

and

$$\mu_L = \mu + \frac{\Delta \mu}{2}, \qquad \mu_R = \mu - \frac{\Delta \mu}{2}. \tag{4.72}$$

Where $\Delta T = T_L - T_R$ and $\Delta \mu = eV$ are applied temperature and voltage bias respectively. We restrict ourselves in the linear response regime such that $k_B T, \Delta\mu << k_B T$. We can expand the distribution function around (μ, T) ,

$$f(T_L, \varepsilon - \mu_L) = f(T, \varepsilon - \mu) + \frac{\Delta T}{2} \frac{\partial f}{\partial T} + \frac{\Delta \mu}{2} \frac{\partial f}{\partial \varepsilon}, \tag{4.73}$$

and

$$f(T_R, \varepsilon - \mu_R) = f(T, \varepsilon - \mu) - \frac{\Delta T}{2} \frac{\partial f}{\partial T} - \frac{\Delta \mu}{2} \frac{\partial f}{\partial \varepsilon}. \tag{4.74}$$

Hence,

$$f(T_L, \varepsilon - \mu_L) - f(T_R, \varepsilon - \mu_R) = \Delta T \frac{\partial f}{\partial T} + \Delta \mu \frac{\partial f}{\partial \varepsilon}. \tag{4.75}$$

Since,

$$\frac{\partial f}{\partial T} = \frac{\varepsilon - \mu}{k_B T^2} \times \frac{\exp\left(\frac{\varepsilon - \mu}{k_B T}\right)}{\left[\exp\left(\frac{\varepsilon - \mu}{k_B T}\right) + 1\right]^2}, \tag{4.76}$$

and

$$\frac{\partial f}{\partial \varepsilon} = -\frac{1}{k_B T} \frac{\exp\left(\frac{\varepsilon - \mu}{k_B T}\right)}{\left[\exp\left(\frac{\varepsilon - \mu}{k_B T}\right) + 1\right]^2}. \tag{4.77}$$

Thus,

$$\frac{\partial f}{\partial T} = -\frac{\varepsilon - \mu}{T} \frac{\partial f}{\partial \varepsilon}. \tag{4.78}$$

Hence,

$$f(T_L, \varepsilon - \mu_L) - f(T_R, \varepsilon - \mu_R) = \frac{\partial f}{\partial \varepsilon} \left(\Delta \mu - \frac{\varepsilon - \mu}{T} \Delta T \right). \tag{4.79}$$

The electric current then reads,

$$I_e = \frac{g_s e}{h} \sum_n \int_0^\infty d\varepsilon T_n(\varepsilon) \frac{\partial f}{\partial \varepsilon} \left(\Delta\mu - \frac{\varepsilon - \mu}{T} \Delta T \right), \tag{4.80}$$

$$= \frac{g_s e}{h} \sum_n \left[\int_0^\infty d\varepsilon T_n(\varepsilon) \frac{\partial f}{\partial \varepsilon} \Delta\mu - \int_0^\infty d\varepsilon T_n(\varepsilon) \frac{\varepsilon - \mu}{T} \frac{\partial f}{\partial \varepsilon} \Delta T \right], \tag{4.81}$$

$$= \frac{g_s e}{h} \sum_n \left(I_1^n \Delta\mu - I_2^n \Delta T \right). \tag{4.82}$$

Where

$$I_1^n = \int_0^\infty d\varepsilon T_n(\varepsilon) \frac{\partial f}{\partial \varepsilon}, \tag{4.83}$$

and

$$I_2^n = \int_0^\infty d\varepsilon T_n(\varepsilon) \frac{\varepsilon - \mu}{T} \frac{\partial f}{\partial \varepsilon}. \tag{4.84}$$

At low temperature,

$$\frac{\partial f}{\partial \varepsilon} = \delta(\varepsilon - \mu). \tag{4.85}$$

Thus,

$$I_1^n = \int_0^\infty d\varepsilon T_n(\varepsilon) \delta(\varepsilon - \mu) = T_n(\mu). \tag{4.86}$$

To evaluate, I_2^n we expand $T_n(\varepsilon)$ around μ,

$$T_n(\varepsilon) = T_n(\mu) + (\varepsilon - \mu) \frac{dT_n(\varepsilon)}{d\varepsilon} |_{\varepsilon=\mu}, \tag{4.87}$$

hence,

$$I_2^n = \int_0^\infty d\varepsilon \left(T_n(\mu) + (\varepsilon - \mu) \frac{dT_n(\varepsilon)}{d\varepsilon} |_{\varepsilon=\mu} \right) \frac{\varepsilon - \mu}{T} \frac{\partial f}{\partial \varepsilon}. \tag{4.88}$$

The first term vanishes by integrating thus,

$$I_2^n = - \int_0^\infty d\varepsilon \left(\frac{(\varepsilon - \mu)^2}{k_B T^2} \right) \frac{\exp\left(\frac{\varepsilon - \mu}{k_B T}\right)}{\left[\exp\left(\frac{\varepsilon - \mu}{k_B T}\right) + 1\right]^2} \times \frac{dT_n(\mu)}{d\varepsilon}. \tag{4.89}$$

If we define,

$$x = \frac{\varepsilon - \mu}{k_B T}, \tag{4.90}$$

then the above equation becomes,

$$I_2^n = - k_B^2 T \int_{-\frac{\mu}{k_B T}}^\infty dx \frac{x^2 \exp x}{(\exp x + 1)^2} \times \frac{dT_n(\mu)}{d\varepsilon}, \tag{4.91}$$

where, $x = -\frac{\mu}{k_B T}$ for $\varepsilon = 0$ and $x = \infty$ when $\varepsilon \to \infty$. In the low temperature limit, $x = -\frac{\mu}{k_B T} \to -\infty$. Hence,

$$I_2^n = -k_B^2 T \int_{-\infty}^{\infty} dx \frac{x^2 \exp x}{(\exp x + 1)^2} \times \frac{dT_n(\mu)}{d\varepsilon}, \tag{4.92}$$

$$= -k_B^2 T \frac{\pi^2}{3} \times \frac{dT_n(\mu)}{d\varepsilon}. \tag{4.93}$$

By plugging the values of I_1^n and I_2^n, in the equation (4.82) and we obtain,

$$I_e = \frac{g_s e^2}{h} \sum_n T_n(\mu) V + \frac{g_s e^2}{h} k_B^2 T \frac{\pi^2}{3} \sum_n \frac{dT_n(\mu)}{d\varepsilon} \Delta T. \tag{4.94}$$

Note that if $\Delta T = 0$, then

$$I_e = \frac{g_s e^2}{h} \sum_n T_n(\mu) V. \tag{4.95}$$

One can read the electrical conductance,

$$G = \frac{g_s e^2}{h} \sum_n T_n(\mu). \tag{4.96}$$

Note that electric current is also driven by the temperature difference, this current generates a voltage across the conductor until the electric current is zero. Thermopower (defined in chapter 2) can be read as,

$$S = \frac{V}{\Delta T} = -g_s \frac{e k_B^2 \pi^2 T}{3Gh} \sum_n \frac{dT_n(\mu)}{d\varepsilon} = -\frac{\pi^2 k_B^2}{3e} \sum_n \frac{d \ln T_n(\mu)}{d\varepsilon}. \tag{4.97}$$

4.6 Thermal current

We describe here thermal current carried by the electrons and we will find the thermal conductance. The entropy current in equation (2.78) is,

$$I_S = \frac{I_E - \mu I_N}{T}. \tag{4.98}$$

In terms of heat current,

$$I_Q = I_E - \mu I_N, \tag{4.99}$$

where $I_Q = TI_S$ and I_E is energy current. If ε is energy of single particle then I_E can be written as, $I_E = \varepsilon I_N$. Hence,

$$I_Q = (\varepsilon - \mu)\, I_N. \tag{4.100}$$

By using the Landauer formula (4.69) we have,

$$I_Q = \frac{g_s}{h} \sum_n \int_0^\infty d\varepsilon T_n(\varepsilon)\,(\varepsilon - \mu)\,\frac{\partial f}{\partial \varepsilon}\left[f(\varepsilon - \mu_L, T_L) - f(\varepsilon - \mu_R, T_R)\right]. \tag{4.101}$$

By using equation (4.79), the above equation can be written as:

$$I_Q = \frac{g_s}{h} \sum_n \int_0^\infty d\varepsilon\,(\varepsilon - \mu)\,T_n(\varepsilon)\frac{\partial f}{\partial \varepsilon}\left(\Delta\mu - \frac{\varepsilon - \mu}{T}\Delta T\right), \tag{4.102}$$

$$= \frac{g_s}{h} \sum_n \left(I_3^n \Delta\mu - I_4^n \Delta T\right). \tag{4.103}$$

Where

$$I_3^n = \int_0^\infty d\varepsilon(\varepsilon - \mu)T_n(\varepsilon)\frac{\partial f}{\partial \varepsilon}, \tag{4.104}$$

and

$$I_4^n = \int_0^\infty d\varepsilon \frac{(\varepsilon - \mu)^2}{T} T_n(\varepsilon)\frac{\partial f}{\partial \varepsilon}. \tag{4.105}$$

For low temperature, I_3^n is already evaluated in equation(4.92),i.e.,

$$I_3^n = \frac{k_B^2 T^2 \pi^2}{3} \times \frac{dT_n(\mu)}{d\varepsilon}. \tag{4.106}$$

We use the expansion of $T_n(\varepsilon)$ to evaluate I_4^n,

$$I_4^n = \frac{1}{T}\int_0^\infty d\varepsilon(\varepsilon - \mu)^2 \left(T_n(\mu) + \frac{dT_n(\varepsilon)}{d\varepsilon}\,|_{\varepsilon=\mu}\right)\frac{\partial f}{\partial \varepsilon}. \tag{4.107}$$

The second term of this integral vanishes by integrating because it contains an odd power of $(\varepsilon - \mu)$. The first term is evaluated similarly as we did earlier in equation (4.92). Hence,

$$I_4^n = -k_B^2 T \frac{\pi^2}{3} T_n(\mu). \tag{4.108}$$

Thus, equation(4.102) becomes,

$$I_Q = -\frac{e g_s}{h}\frac{k_B^2 T^2 \pi^2}{3}\sum_n \frac{dT_n(\mu)}{d\varepsilon} V + \frac{g_s}{h}\frac{k_B^2 \pi^2}{3} T \sum_n T_n(\mu)\Delta T. \tag{4.109}$$

Note that heat current is also driven by the voltage bias as well as temperature bias. The heat current driven by the voltage bias term contribute very small to the thermal conductance so we ignore this term while calculating thermal conductance. Hence,

$$I_Q = g_s \frac{k_B^2 \pi^2}{3h} T \sum_n T_n(\mu) \Delta T. \tag{4.110}$$

One can read the thermal conductance,

$$G_Q = T g_s L_0 \sum_n T_n(\mu), \tag{4.111}$$

where, L_0 is thermal conductance quantum defined as,

$$L_0 = \frac{k_B^2 \pi^2}{3h}. \tag{4.112}$$

Hence, the thermal conductance is quantized in the unit of L_0.

The Peltier coefficient is defined as,

$$\Pi = \frac{I_Q}{I_e}, \tag{4.113}$$

where, I_Q and, I_e are driven by purely voltage bias. Thus,

$$\Pi = -g_s \frac{e k_B^2 \pi^2 T^2}{3Gh} \sum_n \frac{dT_n(\mu)}{d\varepsilon} = -g_s \frac{k_B^2 \pi^2}{3h} T^2 \sum_n \frac{d \ln T_n(\mu)}{d\varepsilon}. \tag{4.114}$$

One can see from equation (4.96) and (4.113) that Π and S are related by the Kelvin Onsager relation

$$\Pi = TS. \tag{4.115}$$

Hence, we convert all transport coefficient in terms of channel and energy dependent transmission coefficient.

Chapter 5

Results and Discussion

The purpose of this work was to provide a brief description of the transport of particles and heat energy in the non-relativistic and ultra-relativistic 2-dimensional electron gas in the low temperature limit where linear response theory works. A viable basis of the Landauer theory in the ballistic transport regime was provided to understand the quantum transport of non-relativistic and ultra-relativistic quasi-free particles and thermal energy carried by these particles. To implement this programme, we developed the concept of thermodynamics. In order to connect the general principle of thermodynamics to the quantum transport, we used the ideas of the Boltzmann theory and ballistically moving charge particles.

Further, we used the Landauer theory to discuss Integer Quantum Hall Effect in low temperature limit(¡1K) and in a high magnetic field limit($\approx 10T$). It was shown that the Hall conductance is quantized by using gauge invariance principle. Moreover, we examined the behavior of a 2-dimensional electron gas that was subjected to both a large perpendicular magnetic field as well as spatially varying internal electric fields. We choose one of the two guiding center coordinates to be diagonal. This made the energy a local function of position, allowing for an easy visualization of the transverse responses to externally imposed fields, as well as the spatial distribution of the (transverse) Hall current inside the sample. Further, in this model, we applied a thermal gradient and calculate the thermal current flowing through the sample which is quantized.

Finally we introduced graphene. It was interesting to see the comparison of ultra-relativistic Dirac particles with the non-relativistic particles. We modified the

Landau formula for this case and applied to calculate electrical and thermal current flowing through a graphene sample. We found here the transport co-efficient in terms of channel dependent transmission co-efficient.

Appendix A

Dirac Hamiltonian

Graphene is made by carbon atoms which are arranged in hexagonal structure. This structure can be viewed as a triangular lattice with a basis of two atoms per unit cell. We start with the tight bonding model approach to understand the band structure of graphene.

The tight binding Hamiltonian with nearest neighbour hopping only is considered here. Consider $a_j^\dagger$ is creation operator which creates an electron on sight $\mathbf{R}_j$ on sub-lattice A and a_j is annihilation operator which annihilates an electron on sub-lattice A. A similar definition can be used for sub-lattice B. The simpler form of tight binding Hamiltonian is

$$H = \varepsilon_0 \sum_i (a_j^\dagger a_j + b_j^\dagger b_j) - t \sum_j \sum_{\delta=1}^{3} (a_{j+\delta}^\dagger b_j + H.C). \tag{A.1}$$

Here, ε_0 is nearest hopping energy. By Fourier transforming the operators, we have,

$$a_j^\dagger = \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{j}} a_{\vec{k}}^\dagger. \tag{A.2}$$

Similarly,

$$b_j^\dagger = \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{j}} b_{\vec{k}}^\dagger. \tag{A.3}$$

Hence,

$$H = \varepsilon_0 \sum_{j\vec{k}\vec{k}'} \left(e^{i(\vec{k}-\vec{k}')\cdot\vec{j}} a_{\vec{k}}^\dagger a_{\vec{k}'} + e^{i(\vec{k}-\vec{k}')\cdot\vec{j}} b_{\vec{k}}^\dagger b_{\vec{k}'} \right) - t \sum_{\delta=1}^{3} \sum_{j\vec{k}\vec{k}'} \left(e^{i(\vec{k}-\vec{k}')\cdot\vec{j}} e^{i\vec{k}\cdot\vec{\delta}} a_{\vec{k}}^\dagger b_{\vec{k}'} + H.C \right). \tag{A.4}$$

Since,

$$\sum_{j} e^{i(\vec{k}-\vec{k}')\cdot\vec{j}} = \delta_{\vec{k}\vec{k}'}. \tag{A.5}$$

Thus,

$$H = \varepsilon_0 \sum_{\vec{k}} \left(a^{\dagger}_{\vec{k}} a_{\vec{k}} + b^{\dagger}_{\vec{k}} b_{\vec{k}} \right) - t \sum_{\vec{k}} \left(f(\vec{k}) a^{\dagger}_{\vec{k}} b_{\vec{k}} + f^{*}(\vec{k}) b^{\dagger}_{\vec{k}} a_{\vec{k}} \right). \tag{A.6}$$

Where,

$$f(\vec{k}) = \sum_{\delta=1}^{3} e^{i\vec{k}\cdot\vec{\delta}}. \tag{A.7}$$

If we define a matrix,

$$H_{\vec{k}} = \begin{pmatrix} \varepsilon_0 & -tf(\vec{k}) \\ -tf^{*}(\vec{k}) & \varepsilon_0 \end{pmatrix}, \tag{A.8}$$

then the above Hamiltonian can be written as

$$H = \sum_{\vec{k}} \begin{pmatrix} a^{\dagger}_{\vec{k}} & a^{\dagger}_{\vec{k}} \end{pmatrix} H_{\vec{k}} \begin{pmatrix} a_{\vec{k}} \\ b_{\vec{k}} \end{pmatrix}. \tag{A.9}$$

We use, $\det(H_{\vec{k}} - \lambda I) = 0$, to find the eigenvalues of the Hamiltonian. Hence,

$$(\varepsilon_0 - \lambda)^2 - t^2 |f(\vec{k})|^2 = 0. \tag{A.10}$$

The solution of the above equation is,

$$\lambda = \varepsilon_0 \mp t|f(\vec{k})|. \tag{A.11}$$

Now we choose our axis in such a way that $\vec{\delta}_1$ makes an angle 60° with the x-axis then,

$$\vec{\delta}_1 = \left(\frac{a}{2}, \frac{\sqrt{3}a}{2} \right). \tag{A.12}$$

Similarly,

$$\vec{\delta}_2 = \left(\frac{a}{2}, -\frac{\sqrt{3}a}{2} \right), \tag{A.13}$$

$$\vec{\delta}_3 = (-a, 0). \tag{A.14}$$

Hence,

$$\begin{aligned} f(\vec{k}) &= \exp(i\vec{k}\cdot\vec{\delta}_1) + \exp(i\vec{k}\cdot\vec{\delta}_2) + \exp(i\vec{k}\cdot\vec{\delta}_3), \\ &= \exp(-ik_x a)\left(1 + 2\exp(3ik_x\frac{a}{2}cos\frac{\sqrt{3}}{2}k_y a)\right). \end{aligned} \tag{A.15}$$

For the physics of graphene, two points are important K and K' near the corners of the (BZ). These are named Dirac points. The coordinates of these points in momentum space are given by

$$\mathbf{K} = \left(\frac{2\pi}{3a}, \frac{2\pi}{3\sqrt{3}a}\right), \qquad \mathbf{K}' = \left(\frac{2\pi}{3a}, -\frac{2\pi}{3\sqrt{3}a}\right). \tag{A.16}$$

We expand $f(\vec{k})$ near these two points in first order to linearise the H_k. By expanding $f(\vec{k})$ near K point we have,

$$\begin{aligned} f(\vec{k}) &= \exp -i(\frac{2\pi}{3a} + k_x)\left(1 + 2\exp(3i(k_x + \frac{2\pi}{3a})\frac{a}{2}cos\frac{\sqrt{3}}{2}(k_y + \frac{2\pi}{3\sqrt{3}a})a)\right), \\ &= -\frac{3a}{2}\exp(2\pi/3)\,(k_x + ik_y)\,. \end{aligned}$$

By restoring $\hbar$ and using equation, $\varepsilon_0 = -tf(\vec{k})$, we obtain,

$$\varepsilon_0 = \hbar v_F(p_x + ip_y). \tag{A.17}$$

Where, $v_F = \frac{3t}{2\hbar a}$.

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