1.1 Introduction

Silicon-metal oxide semiconductor field effect transistors (Si-MOSFETs) are the key components and building blocks of modern electronics. The silicon industry has tremendously grown during the last four decades due to their applications in products like microprocessors, memories, logic devices and many others. One of the important features is the rapid miniaturization of Si-MOSFETs which is described by Moore’s law. Present day processors with billions of MOSFETs with sizes of several tens of nanometers are produced in large scale. However, Moore’s law cannot continue forever as further reduction in size could deteriorate performance of the devices. The problems may be increased power consumption, leakage of current due to thin gate dielectric and tunnelling current between the source and the drain. The miniaturization at the atomic level may lead to failure of Moore’s law and Si-MOSFETs approach a limit in size. Hence, new materials are required to ensure the continuous improvement of the performance of the electronic devices. Recently, carbon based materials have become such one of the important and attractive ones.

Since the invention of carbon nanotube in 1991 [1.1], intense research activity is going on in hexagonally arrayed graphitic carbon systems. Graphene, an isolated two-dimensional (2D) atomic plane of graphite, is the building block for the other graphitic materials such as graphite (stacked graphene), one-dimensional carbon nanotube (rolled graphene) and fullerenes (wrapped graphene) (Figure 1.1). During the last nearly one decade graphene has occupied the centre stage of the condensed matter physics.

![Figure 1.1. Graphitic materials in different dimensions: (a) 0-dimensional fullerene, (b) 1-dimensional carbon nanotube, (c) 2-dimensional graphene and (d) 3-dimensional graphite.](image)

For many decades, free standing graphene layer, as an ideal 2D crystal of carbon atoms, was considered to be thermodynamically unstable due to the thermal
fluctuations causing the lattice distortions or defects [1.2, 1.3]. And hence graphene was studied simply as a theoretical model. In 1946, Wallace [1.4] developed the tight binding theory of band structure of graphene and demonstrated its unusual properties.

The experimental discovery of graphene in 2004 by Novoselov and Geim [1.5], by mechanical exfoliation from graphite, came as a great surprise and they were awarded Nobel prize in physics in 2010 ‘for ground breaking experiments regarding the two-dimensional material graphene’. This discovery gave birth to the new shining star with its exciting properties and a new era for condensed matter physics has begun. Since this discovery, there is explosion of research activity and publications in the field of graphene based structures. Gaphene is a material of great interest not only for the fundamental research but also of enormous technological applications. Due to the special symmetry of honey comb lattice, the electrons behave like a massless relativistic particles, at low energy, leading to the observation of variety of totally new quantum mechanical effects such as novel relativistic (half integer) Quantum Hall effect [1.6-1.8], Klein tunneling [1.9], finite conductivity at zero charge carrier concentration [1.6] and universal minimum conductivity of the order of $e^2/h$ [1.6]. The major breakthrough is that the predicted ‘massless Dirac Fermions’ are experimentally observable and bring quantum relativistic experiment to table top at room temperature.

For future applications point of view, graphene is believed to be a good post-silicon material with silicon based technology almost reaching a fundamental limit. Novoselov and Geim [1.10], University of Manchester, fabricated smallest transistor in the world from graphene. IBM has demonstrated 100 GHz transistor using large area graphene [1.11]. Samsung has made touch screen by garphene [1.12]. Optoelectronics is a field in which graphene can be used on a commercial scale soon. Currently, indium tin oxide is the widely used material in fabrication of optoelectronic devices such as LCD touchscreens for smart phones, tablet and desktop computers and televisions. Since graphene offers significantly high electrical conductivity, almost complete transparency to light, very high tensile strength and flexibility make it as an inevitable candidate in optoelectronic devices. Also graphene is a material that can be utilized in numerous other disciplines including, energy storage, bioengineering and composite materials [1.13].
Graphene has shown highest ever intrinsic carrier mobility \( > 10^5 \text{ cm}^2/\text{Vs} \) at room temperature [1.14, 1.15], which is nearly 100 times larger than in the present silicon devices. Consequently, it finds applications in high speed devices.

1.2 Scope of the present work

Although intensive studies have been carried out on the electronic structure and transport properties of graphene-based materials [1.16, 1.17], there are still many important issues that need to be understood. The main aim of this study is to understand and investigate some of the thermoelectric and electrical transport properties, namely thermopower and transport in high electric field.

Thermopower \( S \), one of the important transport properties, finds applications in thermoelectric power generation and thermoelectric coolers. A high value of thermoelectric figure of merit \( ZT \ (\sim S^2) \) is an indicative of efficient thermal energy harvesting mechanism. Obtaining maximum value of \( S \) is one of the ways to maximize \( ZT \). Besides, thermopower provides information of electronic structure and physical processes involved in the transport phenomena.

High electric field transport includes hot electron energy relaxation studies which provide insight into the thermal link between electrons and phonons. Electron heating by photons finds potential applications in bolometry and calorimetry. In order to look for the applications in high current circuits and devices it is essential to know the behavior of graphene in non-linear current-field characteristics. Particularly, behavior in the current saturation regime is important where analog amplifiers operate. In graphene transistors, the achievement and control of saturation velocity of electron in high electric field is crucial for analog devices. The investigation of these properties including the hot phonon effect will bring out some new features.

In the present work (i) thermopower and (ii) high electric field transport properties are investigated in two graphene based structures, namely, (i) bilayer graphene and (ii) graphene nanoribbon. Thermopower is studied in Part-A and high field transport is studied in Part-B of the thesis.

In the remaining part of this chapter, lattice structure and electronic structure of monolayer graphene, bilayer graphene and graphene nanoribbons are given. This is followed by the description of different scattering mechanisms that limit the transport properties in these systems.
1. 3. Lattice structure of graphene structures

1.3.1 Monolayer graphene

Monolayer graphene (MLG) can be viewed as an individual plane of carbon atoms extracted from graphite. It is made up of carbon atoms arranged in hexagonal honeycomb like lattice structure, as shown in the Figure 1.2.

![Figure 1.2. Atomic plane of MLG from 3-dimensional graphite.](image)

A carbon atom has six electrons, occupying the atomic orbitals $1s^2$, $2s^2$ and $2p^2$. The outer four electrons being at $2s$ and $2p$ states, have similar energies and three of them are $sp^2$ hybridized. These three electrons lie in the $xy$-plane with a separating angle of 120° form $\sigma$ bonds with their neighbors and give rise to the hexagonal lattice structure of graphene. The remaining electron is in $\pi$ state and aligned in the $z$-direction. This delocalized electron is weakly bonded, has low energy of excitation. It can hop easily between neighboring atoms and is the main cause for the transport properties of graphene. One conduction electron is contributed from each atom and three strong covalent bonds with its nearest neighbors. These strong bonds give the mechanical strength to one atom thick graphene sheet and making it possible to be freely suspended [1.18].

![Figure 1.3. $sp^2$ hybridization of carbon atoms in graphene.](image)
The honeycomb lattice can be described as two interpenetrating triangular sublattices A and B shown in Figure 1.4 (a). The structure can be seen as a triangular lattice with a basis of two atoms per unit cell. These two equivalent lattice sites A and B in the 2D hexagonal lattice give rise to the ‘chiral’ property to the carriers.

Figure 1.4. (a) Lattice structure of MLG with A and B lattice, (b) reciprocal lattice [1.16].

The two primitive lattice vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ can be written as [1.16]

$$\mathbf{a}_1 = \frac{a}{2}(3, \sqrt{3}), \quad \mathbf{a}_2 = \frac{a}{2}(3, -\sqrt{3}),$$

(1.3.1)

where $a = |\mathbf{a}_1| = |\mathbf{a}_2| = 2.46$ Å is the lattice constant, 1.42 Å is the carbon-carbon bond length in graphene [1.19]. The reciprocal lattice vectors are given by

$$\mathbf{b}_1 = \frac{2\pi}{3a}(1, \sqrt{3}), \quad \mathbf{b}_2 = \frac{2\pi}{3a}(1, -\sqrt{3}).$$

(1.3.2)

The reciprocal lattice is a hexagonal Bravais lattice and it is shown in Figure 1.4 (b).

1.3.2 Bilayer graphene

Figure 1.5. Atoms A1 and B1 on the lower layer are shown as white and black circles; A2, B2 on the upper layer are black and grey, respectively, and $\gamma_i$'s are the inter layer hopping parameters.
Bilayer graphene (BLG) is a coupled two monoatomic layers of graphene, separated by 0.34 nm, each with a honeycomb crystal structure. The primitive cell lattice vectors $a_1$ and $a_2$ and the reciprocal lattice vectors $b_1$ and $b_2$ are same as that of the MLG.

Bilayer graphene consists of four atoms in the unit cell, labeled A1, B1 and A2, B2 on the lower and upper layer, respectively. The layers are arranged so that one of the atoms from the lower layer B1 is directly below an atom A2 from the upper layer. The atomic sites B1 and A2 are referred as ‘dimer’ sites because the electronic orbitals of them are coupled together by a relatively strong interlayer coupling. The other two atoms, A1 and B2, don’t have a counterpart on the other layer that is directly above or below them, and are referred to as ‘non-dimer’ sites [1.20].

1.3.3 Graphene nanoribbons

Graphene nanoribbons (GNRs) are stripes of graphene with ultra-thin width. The strip of graphene of length $L$ and finite width $W$ can be viewed as a new class of quasi-one-dimensional wire, in which carriers are free to move only along its length. The primitive cell lattice vectors $a_1$ and $a_2$ and the reciprocal lattice vectors $b_1$ and $b_2$ are same as that of the MLG. There are two basic shapes for graphene edges: armchair and zigzag. The lattice structures of the armchair and zigzag nanoribbons are shown in Figure 1.6.

Figure 1.6. Lattice structure of armchair and zigzag graphene nanoribbons

In the zigzag graphene nanoribbon (ZGNR) the atoms at each edge belong to the same sublattice A, and in armchair graphene nanoribbon (AGNR) the edge consists of lines of A-B dimers. The width of the nanoribbon is approximately given by $W = (N/4)a$ and $W = (N/4)\sqrt{3}a$, respectively, for armchair and zigzag nanoribbon, where $N$ is the number of atoms per unit cell. GNRs with armchair edges on both
sides are metallic or semiconducting; zigzag edges on both sides are always metallic with peculiar localized states at both the edges \[1.21\]. Graphene nanoribbons can be experimentally produced by using lithography techniques and chemical techniques \[1.22, 1.23\].

1.4 Energy states of carriers in graphene structures

1.4.1 Monolayer graphene

The tight binding theory of band structure of graphene is developed by Wallace \[1.4\]. The electronic properties of low energy electrons, near the Dirac point, are of interest for electronic transport. The long wavelength low energy effective 2D continuum Schrödinger equation for graphene carriers is given by \[1.16, 1.17\]

\[
\hbar v_f \mathbf{k} \cdot \mathbf{\sigma} \psi_k (\mathbf{r}) = E_k \psi_k (\mathbf{r}),
\]

where \(\mathbf{\sigma} = (\sigma_x, \sigma_y)\) are the Pauli matrices, \(E_k\) is the energy eigen value, \(\psi_k (\mathbf{r})\) is the 2D wave function, \(k(\mathbf{r})\) is the 2D wave (position) vector and \(v_f\) is the Fermi velocity. In momentum space, the corresponding Hamiltonian is

\[
H = \hbar v_f \begin{pmatrix} 0 & k_x - i k_y \\ k_x + i k_y & 0 \end{pmatrix} = \hbar v_f \mathbf{k} \cdot \mathbf{\sigma}.
\]

The wave function, in momentum space, around \(K\) is given by \[1.24\]

\[
\psi^K_{xk}(\mathbf{r}) = e^{i k \cdot \mathbf{r}} \phi^s_{k} / \sqrt{A},
\]

where

\[
\phi^s_{k} = (e^{-i \theta _k}, s),
\]

\(s = +1\) for the conduction band (electrons) and \(-1\) for valance band (holes), \(\tan \theta_k = k_y / k_x\) and \(A\) is the area of the graphene. The corresponding energy eigen value is given by

\[
E_k = \pm \hbar v_f k.
\]

Hence, graphene is a zero, direct band gap 2D semiconductor with linear energy dispersion for both electrons and holes which are 2D in nature. In Figure 1.7, we have shown the band structure of graphene at both \(K\) and \(K'\) points in the Brillouin zone. The dispersion relation matches with that of Dirac’s relativistic electron with zero rest mass. Hence carriers are called Dirac particles in graphene and their effective band mass is zero. The points (\(K\) and \(K'\)) at which conduction band and valance band meet
are called ‘Dirac points’ or ‘charge neutrality points (CNP)’. The existence of two Dirac cones for electrons and holes, touching each other in momentum space, gives rise to a valley degeneracy $g_v=2$.

![Graphene Band Structure](image)

**Figure 1.7.** (a) Electronic band structure of graphene obtained using tight-binding approximation, (b) band structure near the Dirac point (c) density of states of graphene close to the Dirac point. The inset shows the density of states over the full electron bandwidth.

The density of states $D(E)$, defined as the number of allowed states in unit energy range per unit area, is given by

$$D(E) = g_s g_v \sum_k \delta(E - E_k),$$

(1.4.11)

where $g_s$ and $g_v$ are the spin and valley degeneracies, respectively; $g_v=g_s=2$ for MLG. Converting the summation to integration, Eqn. (1.4.11) gives

$$D(E) = \frac{g_s g_v}{2\pi \hbar^2} \left( \frac{E}{v_f} \right)^2$$

(1.4.12)

which shows $D(E) \sim E$ (Figure 1.7(c)).
1.4.2 Bilayer graphene

Electronic properties of BLG, which is an intermediate between monolayer and a graphite system, can be studied by using the descriptions of the tight binding approximations [1.16, 1.25].

![Figure 1.8](image)

**Figure 1.8.** (a) Band structure of BLG near Dirac point. (b) The energy band close to the neutrality point K is shown enlarged for different values of applied potential $V$ [1.16, 1.27], (c) density of states near the Dirac points.

In BLG, the interlayer coupling leads to massive quasiparticles unlike zero effective mass of the carriers in MLG. The long wavelength, low energy effective 2D continuum Schrödinger equation for bilayer graphene carriers near the Dirac point is given by [1.25, 1.26]

$$ H\psi_k(r) = E_k\psi_k(r) $$

(1.4.13)

with the Hamiltonian

$$ H = -\frac{\hbar^2}{2m} \begin{pmatrix} 0 & (k_x - ik_y)^2 \\ (k_x + ik_y)^2 & 0 \end{pmatrix}, $$

(1.4.14)
where $m=0.033m_0$ is the effective mass of the carriers. The corresponding eigen function in momentum space around $K$ is given by

$$\psi^K_{s,k}(r) = e^{ikr} \phi_{k_s} / \sqrt{A},$$

where

$$\phi_{k_s} = (e^{-2i\theta_k}, s) / \sqrt{2}$$

with the energy eigen value

$$E_k = \pm \hbar k^2 / 2m.$$

Here $k = ke^{i\theta_k}$ is the 2D electron wave vector, and $\theta_k = \tan^{-1}(k_y/k_x)$ as in MLG. Hence, BLG is a zero band gap semiconductor with parabolic dispersion in the neighborhood of Dirac points. However, in BLG energy gap can be created and tuned by application of external electric field as shw in Figure 1.8 (b) [1.27].

The density of states corresponding to low energy region is given by [1.17]

$$D(E) = \frac{g_s g_v m}{2\pi \hbar^2}.$$  (1.4.18)

The $D(E)$ as a function of energy is shown in Figure 1.8 (c) for $g_v = g_s = 2$.

### 1.4.3 Graphene nanoribbons

In graphene nanoribbon electronic structure is determined by their edge shapes and width. For the low energy states near $K$ and $K'$, $k \cdot p$ approximation is adopted to describe electronic structure of GNRs [1.16,1.21, 1.28,1.30].

#### 1.4.3.1 Armchair graphene nanoribbon

We consider an armchair graphene nanoribbon with length $L$ along $y$- axis and width $W$ along $x$- axis. The wave functions are expressed in terms of envelope functions $[\psi_A(r), \psi_B(r)]$ and $[\psi'_A(r), \psi'_B(r)]$. The envelope functions may be combined into a four-vector $\Psi = (\psi_A(r), \psi_B(r), -\psi'_A(r), -\psi'_B(r))$ which satisfies a Dirac equation $H\Psi = E\Psi$, with the Hamiltonian [1.28]

$$H = \hbar v_f \begin{pmatrix}
0 & -k_x + ik_y & 0 & 0 \\
-k_x - ik_y & 0 & 0 & 0 \\
0 & 0 & 0 & k_x + ik_y \\
0 & 0 & k_x - ik_y & 0
\end{pmatrix}.$$ (1.4.19)
The corresponding wave function is derived using the admixture states in the K and K' valleys. Since, in AGNR, K and K' are projected on the same point of the 1D Brillouin zone, the confined states emerge only from a Dirac point K = K'. For semiconducting armchair GNRs the valley degeneracy is removed (g=1). The electronic wave function to satisfy hard boundary conditions

\[ \psi'_{k_n,k_y}(r) = \psi_{k_n,k_y}(r) - \psi'_{k_n,k_y}(r) / \sqrt{2}, \]  

and

\[ \psi_{k_n,k_y}(r) = \frac{1}{\sqrt{2LW}} e^{ik_yy} e^{i[(\Delta K/2) - k_n]y} \left( e^{i\theta_{n,k_y}} - e^{-i\theta_{n,k_y}} \right), \]

with \( \Delta K = 4\pi/3a \). The corresponding energy eigen value for armchair graphene nanoribbon is

\[ E_{k_n,k_y} = \hbar v_f \sqrt{k_n^2 + k_y^2}, \]

where

\[ k_n = \frac{2\pi n}{2W + a} + \frac{2\pi n}{3a}, \]

\( k_y \) is the electron wave vector along y-direction, \( n = 0, \pm 1, \pm 2, \pm 3 \ldots \) and \( \theta_{n,k_y} = \tan^{-1}(k_y/k_n) \). Thus, the motion of the carrier is free in y-direction and it is confined in the x-direction leading to the quantization of energy in the direction of confinement.

Note, if ribbon consists of 3M+1 atoms (M is an integer) \( W= (3M+1)a \), the allowed values of the \( k_n = (2\pi/3a)\left[(2M +1+n)/(2M +1)\right] \) create a doubly degenerate states for \(|2M+1+n|\geq 0\). Then, zero energy solutions are allowed as \( k_y \to 0 \). This kind of ribbon is called metallic. Otherwise, the nanoribbons have nondegenerate states and do not have zero energy mode. These nanoribbons possess energy gap i.e. the ribbons are semiconducting or insulating (Figure 1.9 (a)). The energy dispersion of semiconducting AGNR is with [1.29, 1.30]
Introduction to graphene structures

\[ k_n = n \pi / 3W, \]  
(1.4.25)

with \( n = \pm 1, \pm 2 \ldots \), showing the inverse dependence of \( E_{k_n,k_y} \) on \( W \). With respect to the width of the nanoribbon, energy of the confined states behaves in a discontinuous way. For semiconducting AGNR the energy gap \( E_g = 2 \pi \hbar v_f / 3W = 1.38 / W \) eV.

\[ W_{vE} \frac{3}{2} = \frac{\eta \pi}{2}, \]  
(1.4.26)

and it is shown in Figure 1.9 (c). Density of states for metallic AGNR is shown in Figures 1.9 (d).

1.4.3.2 Zigzag graphene nanoribbon

The Hamiltonian for the zigzag graphene nanoribbon can be obtained from that of AGNR by rotation of the system by an angle \( \pi / 2 \) i.e. changing \( k_x \rightarrow k_y \) and \( k_y \rightarrow -k_x \) [1.16, 1.28]. The boundary conditions at the edge of the nanoribbon (at \( y = 0 \) and \( y = W \)), are \( \Psi_{k_n,k_x} (x,0) = 0 \) and \( \Psi_{k_n,k_x} (x,W) = 0 \). These boundary conditions lead to an energy eigen value of the form

**Figure 1.9.** Energy bands for armchair nanoribbons with (a) \( W = 24a \) and (b) \( W = 25a \) atoms in the unit cell [1.21]. (c) density of states of the semiconducting AGNR for \( N=4 \) and (d) metallic AGNR for \( N=5 \) [1.31].

The corresponding density of states for semiconducting AGNR is given by [1.30]

\[ D(E_{k_n,k_y}) = \frac{2}{\pi \hbar v_f} \frac{E_{k_n,k_y}}{\sqrt{E_{k_n,k_y}^2 - \frac{E_n^2}{2}}}, \]  
(1.4.26)

and it is shown in Figure 1.9 (c). Density of states for metallic AGNR is shown in Figures 1.9 (d).
where \( z \) is obtained from the transcendental equation \( \tanh(zW) = z/k_x \). The transverse and longitudinal components of the wave vector are coupled in ZGNR, in contrast to AGNR. For real values of \( z = k_n \) the solutions correspond to the surface states. Pure imaginary value \( z = ik_n \) leads to \( k_x = k_n / \tan(k_n W) \). The solutions of this equation correspond to the confined modes of the ZGNR.

The corresponding density of states will have the same form as that of AGNR with \( k_y \) replaced by \( k_x \) i.e.

\[
D(E_{k_n,k_x}) = \frac{2}{\pi \hbar f} \frac{E_{k_n,k_x}}{\sqrt{E_{k_n,k_x}^2 - E_n^2}}.
\]

\[\text{(1.4.28)}\]

**Figure 1.10.** Energy bands for a zigzag nanoribbon with 56 atoms in the unit cell. \( k_x \) is the wave vector parallel to the nanoribbon. The dispersionless states correspond to confined edge states. This Brillouin zone is shifted \( \pi/a \) with respect the zigzag Brillouin zone [1.21].

### 1.5 Scattering mechanisms in graphene structures

Central to the understanding of electronic transport properties of graphene is the mechanisms causing the scattering of its charge carriers. The presence of scattering in any system is inevitable. As in conventional semiconductors, transport properties of graphene system are also limited by both disorder (impurities and defects) and lattice (phonons) scattering [1.30, 1.32–1.39]. In this section we describe and discuss the various scattering mechanisms influencing the transport properties in different graphene structures.
Due to the connections between atoms, the displacement of one or more atoms from their equilibrium positions causing lattice deformations in turn gives rise to 2D lattice waves. Depending on the frequency of vibrations they are classified as the acoustic and optical branches. Phonons are 2D in nature. Graphene is also curious from the phonon point of view with large optical phonon energy of 160–200 meV and a weak coupling of electrons to acoustic phonons [1.30, 1.32, 1.34, 1.35, 1.40-1.43]. Phonons are the intrinsic source of scattering in disorder free graphene limiting its intrinsic resistivity and mobility. There are in-plane and out-of-plane (flexural) acoustic phonons. The latter are important only in suspended graphene. In the present study the in-plane acoustic phonons are considered.

1.5.1 Acoustic phonon scattering

The dominant form of electron-phonon coupling for long wavelength acoustic phonon modes is due to deformation potential coupling [1.30, 1.34, 1.35]. For in-plane modes, the potential due to propagation of acoustic phonons is of the form $D \nabla \cdot \textbf{u}(\textbf{r})$, where $\textbf{u}(\textbf{r})$ is the displacement vector and $D$ is the acoustic deformation potential constant. The deformation potential coupling is nonzero only for LA modes. Thus we may use the expansion in terms of longitudinal plane wave $\textbf{u}(\textbf{r}) = \sum_q u_q e^{i(\textbf{q} \cdot \textbf{r})}$, with $u_q = i(\hbar^2/2\rho A \omega_q)^{1/2}(b_q + b_q^*)$, where $b_q$ and $b_q^*$ are phonon annihilation and creation operators, respectively, $\omega_q = v_q \textbf{q}$ is the frequency of the acoustic wave with the wave vector $\textbf{q}$, $v_q$ is the velocity of the phonons, and $\rho$ is the areal mass density of the graphene.

From the scattering potential and the electron states, the matrix elements, for different graphene structures, for the scattering of electrons from initial state $\textbf{k}$ to final state $\textbf{k'}$ due to acoustic phonons via deformation potential coupling, are given by [1.30,1.33, 1.34]

\begin{align*}
|M(\textbf{k}, \textbf{k}')|^2 &= (\hbar D^2 q / 2 \rho A v_y) g(\theta_{\textbf{k} \textbf{k}'}) \quad \text{MLG} \quad (1.5.1) \\
|M(\textbf{k}, \textbf{k}')|^2 &= (\hbar D^2 q / 2 \rho A v_y) g(\theta_{\textbf{k} \textbf{k}'}) \quad \text{BLG} \quad (1.5.2) \\
|M(\textbf{k}, \textbf{k}')|^2 &= (\hbar D^2 q / 2 \rho L W v_y) g(\theta_{n_k, k; n', k'}) \quad \text{AGNR.} \quad (1.5.3)
\end{align*}
Here, $\theta_{kk'} = \theta_k - \theta_{k'}$ is the angle between $k$ and $k'$ and $g(\theta_{kk'}) = |\phi_{k_x}^n^*\phi_{k'_y}|^2$ is the overlap function arising due to spinor wave function $\phi_{k_x}$. Their respective forms are given by
\[
g(\theta_{kk'}) = (1 + \cos \theta_{kk'})/2 \quad \text{MLG} \quad (1.5.4)
\]
\[
g(\theta_{kk'}) = (1 + \cos 2\theta_{kk'})/2 \quad \text{BLG} \quad (1.5.5)
\]
\[
g(\theta_{n,k_x;n',k'_y}) = (1 + \cos \theta_{n,k_x;n',k'_y})/2 \quad \text{AGNR}. \quad (1.5.6)
\]

### 1.5.2 Non-polar optical phonon scattering

Optical phonons are the dominant source of carrier scattering at higher temperatures ($> 300$ K). The Hamiltonian for the electron-optical phonon interaction is given by $H_{op} = u(r)D_{op}$, where $D_{op}$ is the optical deformation field. Thus, we may use the expansion in terms of longitudinal plane wave
\[
u(r) = \sum_q (\hbar^2 / 2\rho A \omega_q)^{1/2} (b_q + b_q^*) e^{i(q \cdot r)} ,
\]
where $b_q$ and $b_q^*$ are the optical phonon annihilation and creation operators and $\omega_q$ is the phonon frequency. From this scattering potential and the wave function the electron-optical phonon interaction matrix element is given by [1.35]
\[
|M(k,k')|^2 = \frac{g(\gamma_1^0)^2 \hbar^2}{2\Lambda \rho \omega_1} g(\theta_{kk'}) \quad \text{MLG} \quad (1.5.7)
\]
\[
|M(k,k')|^2 = \frac{g(\gamma_1^0)^2 \hbar^2}{2\Lambda \rho \omega_1} g(\theta_{kk'}) \quad \text{BLG} \quad (1.5.8)
\]
Here $\gamma_1$'s are the inter layer hoping parameters, $\gamma_1^0 \approx 40eV$, $\gamma_1 \approx 0.4eV$, and
\[
g(\theta_{kk'}) = [1 - s_\alpha s_\beta \cos(\theta_k + \theta_{k'} - 2\theta_\alpha)]/2 \quad \text{MLG.} \quad (1.5.9)
\]
and
\[
g(\theta_{kk'}) = ((hv)^2 / \gamma_1) \{k^2 + k'^2 + 2k'k [\pm \cos(\theta_{kk'}) - s_\alpha s_\beta \cos(\theta_{k_\alpha} + \theta_{k_\beta})] \}
\]
\[
\pm s_\alpha s_\beta (k^2 \cos(2\theta_{k_\alpha}) + k'^2 \cos(2\theta_{k_\beta}))/2, \quad \text{BLG} \quad (1.5.10)
\]
The vector $\hat{a} = \hat{q}(\hat{z} \times \hat{q})$ for longitudinal (transverse) optical branch, $\hat{z}$ is normal to the graphene plane, $\alpha$ and $\beta$ are chosen such that $s_\alpha = \text{sign}(x)$ and $s_\beta = \text{sign}(x - 1)$ and the interval $0 < x < 1$ corresponds to interband scattering.

In AGNR the perturbation potential introduced by LO phonons is given by [1.30]
Introduction to graphene structures

\[ V_{op}(y) = \frac{\hbar}{2\rho LW\omega_{op}} D_{op} e^{iq_y y}. \]  
\hfill (1.5.11)

The corresponding matrix element is given by

\[ |M(k, k')|^2 = \frac{\hbar D_{op}^2}{2\rho L W \omega_{op}} g(\theta_{n, k_y; n', k_y'}), \]  
\hfill (1.5.12)

where \( g(\theta_{n, k_y; n', k_y'}) \) is same as in the case of acoustic phonons in AGNR.

1.5.3 Surface polar phonon scattering

In polar substrates such as SiO\(_2\), vibrations of this substrate ions with the opposite charge polarity give rise to 2D surface polar phonons. A nonvanishing electric field which decays exponentially from the surface of the substrate is generated by the propagation of surface phonon modes. The interaction of these surface polar phonon modes with charge carriers in the conduction channel, due to their close proximity with the underlying substrate, renders the more prominent scattering due to these modes.

The Hamiltonian of electron-surface polar phonon modes is given by [1.37]

\[ H = eF \sum_{q} \left[ e^{-qz} (e^{iq_x} b_q + e^{-iq_x} b_q^+) \right] \sqrt{q}, \]  
\hfill (1.5.13)

where

\[ F^2 = \left( \frac{\hbar \omega_s}{2 A \epsilon_0} \right) \left[ (\epsilon_x + 1)^{-1} - (\epsilon_s + 1)^{-1} \right] , \]  
\hfill (1.5.14)

\( \epsilon_x^\infty (\epsilon_0^\infty) \) is the high (low) frequency dielectric constant of the substrate and \( \hbar \omega_s \) is the energy of surface polar phonons. The corresponding electron-surface phonon interaction matrix element is given by [1.37-1.39]

\[ |M(k, k')|^2 = e^2 F^2 \left( e^{-2qd / q} \right) g(\theta_{kk'}), \]  
\hfill (1.5.15)

MLG

\[ |M(k, k')|^2 = e^2 F^2 \left( \left[ e^{-2qd} + e^{-2q(d+c)} \right] / 2q \right) g(\theta_{kk'}), \]  
\hfill (1.5.16)

BLG

\[ |M(k, k')|^2 = (\hbar D_{op}^2 / 2 \rho Wh \omega_s) g(\theta_{n, k_y; n', k_y'}), \]  
\hfill (1.5.17)

AGNR

where \( g(\theta_{kk'}) \) is same as that in case of acoustic phonon scattering for all the systems, \( d \) is the distance between the graphene and substrate and \( c \) is the inter layer distance.
1.5.4 Charged impurity scattering

The scattering by charged impurity centers, located near the interface between the graphene layer and the substrate, is the most likely scattering mechanism that limit the transport in graphene. This interaction is screened by conduction electrons.

The matrix element of the scattering potential of randomly distributed screened impurity charge centers in MLG is given by [1.44]

\[
|M(k,k')|^2 = \left| \frac{v_i(q)}{\epsilon(q)} \right|^2 g(\theta_{kk'}) ,
\]

where \(v_i(q) = 2\pi^2 q/q e\) is the Fourier transform of the 2D Coulomb potential in an effective background lattice dielectric constant \(\epsilon\). \(\epsilon(q) = \epsilon(q,T)\) is the temperature dependent static 2D screening function given by \(\epsilon(q,T) = 1 + \epsilon_c(q)\Pi(q,T)\), where \(\Pi(q,T)\) is the graphene irreducible finite-temperature polarizability function and \(\epsilon_c(q)\) is the Coulomb interaction.

In case of BLG, the matrix element of the scattering potential is same as that in MLG with the screening function \(\epsilon(q) = 1 + (q_{TF}/q)\) [1.36] and \(q_{TF} = 4m^2/\hbar^2\) is the Thomas-Fermi screening wave vector.

The unscreened Coulomb potential due to charged impurity in an AGNR is given by [1.30]

\[
V(x_0, y, z) = e^2 / 4\pi\epsilon_0\kappa\sqrt{d^2 + y^2} ,
\]

where \(z\) is the distance of the impurity from the AGNR plane, \(\kappa = (\epsilon_r+1)/2\) is average relative dielectric constant of materials on the two sides of the AGNR, \(\epsilon_r\) is the dielectric constant of the substrate, \(d\) is the distance of the impurity atom from the origin. The screened impurity perturbation matrix element is then given by

\[
V(q_y) = \frac{e^2}{2\pi\epsilon_0\kappa e_{scr}} \frac{1}{LW} \int_0^W dK_0(|\Delta k_y| d)dxg(\theta_{n,k_y,n',k_y}) ,
\]

where \(\Delta k_y = k_y - k_y'\) is the change in the carrier wave vector along the GNR axis upon scattering, \(K_0(x)\) is the zeroth-order modified Bessel function, and \(e_{scr}\) is the screening factor. In long wavelength limit, it is given by

\[
e_{scr} \approx 1 + (e^2 / 2\pi\epsilon_0\kappa)\rho_{GRN} (E_F) \ln(2/q_yW) .
\]
1.5.5 Short-range disorder

The matrix element of the scattering potential is determined by the configuration of the 2D systems and the spatial distribution of the point defects. For short-range disorder (defect), we have \[ |M(k,k')|^2 = V_0^2 g(\theta_{kk'}) , \quad (1.5.22) \]
where \( V_0 \) is a constant short-range potential strength. This matrix element is taken to be same for both MLG and BLG with appropriate \( g(\theta_{kk'}) \).

1.6 Scattering rate and relaxation time

The expression for the relaxation times for the above-mentioned scattering mechanisms may be obtained from the scattering rate, being derived using first order time-dependent perturbation theory

\[ P(k,k') = \frac{2\pi}{\hbar} |M(k,k')|^2 \delta(E_k - E_k' \mp \hbar \omega_q) \delta_{k,k'\pm q} . \quad (1.6.1) \]

Here, \( E_k \) and \( E_{k'} \) are the energies of the carrier in the initial and final states related by the condition of momentum conservation \( k' = k \pm q \). Dirac delta function ensures energy conservation in the scattering process. If the scattering is associated with the harmonic time-dependent perturbation such as the normal modes of crystal lattice with frequency \( \omega_q \), then \( \hbar \omega_q \) appears in the Dirac delta function with \( \pm \) referring to absorption and emission of phonons, respectively. The scattering rates due to various mechanisms can be obtained by using the respective matrix elements. The momentum relaxation time is related to the transition probability by

\[ \frac{1}{\tau(E_k)} = \sum_{k'} P(k,k')(1 - \cos \theta_{kk'}) . \quad (1.6.2) \]
Introduction to graphene structures

References

Introduction to graphene structures