University of Nevada, Reno

# Quantum Transport of Electrons through Graphene and Carbon Nanotubes

A dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Physics

by

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May, 2013



#### THE GRADUATE SCHOOL

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#### Quantum Transport of Electrons through Graphene and Carbon Nanotubes

be accepted in partial fulfillment of the requirements for the degree of

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### Abstract

Quantum transport of electrons through graphene has attracted increased interest in the field of nano-technology. Quantum transport through mesoscopic systems explains a wide range of interesting experimental findings, such as: rectification, switching mechanism and transistor actions. We focused our research on the quantum transmission of electrons through graphene and carbon nanotubes. Graphene and nanotube devices operated between source and drain shows a peculiar negative differential resistance behavior (NDR) while drawing current- voltage characteristics. This property is used in many electronic devices. The main feature of graphene is that the electron has zero effective mass at Dirac points, but gains mass when the graphene sheet is folded into a nanotube. Scientists have analyzed the vanishing mass of the electron inside graphene and explain the observed mass gain through Higgs mechanism. We focus our study on the Klein Paradox which deals with the reflection probability greater than one as well as a negative transmission probability. This has been predicted by Oscar Klein and remained a mystery until 1929; the Klein Paradox finally was proven with experimental and theoretical evidence by Geim and Novoselov. In the case of graphene, conductivity is an exponential function of temperature, whereas nanotubes follow a power law. This is a very characteristic feature of quantum dots.

## Acknowledgement

From the bottom of my heart, I would like to express my sincere gratitude to my advisor Dr. Peter Winkler and I would also like to express my deep appreciation for his great help and encouragement which has been extremely valuable for my Ph.D. I appreciate his great time and devotion. His knowledge and constructive way of thinking has become a great pillar of my dissertation. I also appreciate Dr. Friedwardt Winterberg for his valuable suggestions and teaching of General Theory of Relativity. I am also grateful to Dr. Alla Safronova for her helpful suggestions and teaching basic concepts quantum mechanics. I also appreciate the helps of Drs. Aaron Covington and David M. Leitner. I would like to thank to Dr. Benny Bach for his conceptual guidance about establishing experimental laboratories. I am so much grateful to my family and especially to my father Late Sri Nitendra Lal Das for teaching me General Theory of relativity. Finally I am so much grateful to all professors for teaching graduate courses and I express my special gratitude to the Department of Physics for providing Teaching Assistantship as well as kind suggestions.

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# 1 Chapter

#### 1.1 Motivations and objectives

Quantum transport of electron pathways has recently attracted increased interest in the field of nano-technology. Quantum transport through mesoscopic systems, i.e., transport through small molecules like fullerene, graphene, nanotubes etc. explain a wide range of interesting experimental findings such as rectification, switching mechanisms and transistor actions. In 1974, the first theoretical proposal for a single molecular rectifier was published by Aviram and Ratner [1], but due to the limitations of technology at that time, it did not receive all of the deserved attention. With the advance of technology, their ideas gradually led to the notion of intramolecular transport phenomena. Molecular electronics, using single molecules as active elements, is now an active technological concept. Molecular devices are considered as promising candidates for the fabrication of smaller, faster and cheaper nano-sized electronic devices in the fields of photoelectric, information technology and material science. Important examples have been studied theoretically and experimentally such as molecular diodes, molecular transistors, molecular logical circuits and atomic switching devices. These days, scientists are interested in the properties of graphene and nanotubes. Graphene was fabricated experimentally by A. K. Geim and Novoselov [2] in 2004 and previously was supposed to not be possible. The main characteristics of graphene are that due to the interaction of electrons with potential of the lattice, its effective mass becomes zero and the transmission coefficient seemed to be independent of barrier width which motivated

me to study relativistic quantum transport phenomena through graphene and nanotubes. The band structure of graphene was derived in 1947 using a tight binding model and Bloch waves, and can be given by the following expression:

$$\Psi_{\vec{k}} = \sum_{\vec{R}} e^{i\vec{k}.\vec{R}} \, \Phi(\vec{x} - \vec{R}), \qquad [1.1.1]$$

where  $\phi$  indicates the one-electron atomic wave functions ( $p_z$  orbitals). The following energy dispersion relation [3] is obtained

$$E(k)^{\pm} = \pm \gamma \sqrt{1 + 4\cos\frac{\sqrt{3}}{2}ak_x \cos\frac{a}{2}k_y + 4\cos^2\frac{a}{2}k_y} \quad .$$
 [1.1.2]

The two solutions correspond to the bonding (-) and anti-bonding (+) orbitals. The two energy bands touch each other at six points at the edges of the Brillouin zone, out of which two pair of points are known as the Dirac points [2] where effective mass of the electron is zero. A peculiarity of graphene is that its charge carriers do not show the typical dispersion relation  $E(k) = \hbar^2 k^2 / 2m^*$ , a characteristic of free electrons in metals and semiconductors, but rather follow a linear dispersion relation  $E(k) \approx \pm \hbar |k| v_F$ . In the vicinity of Dirac points, Fermi velocity is [4]  $v_F = 10^6 m/s$ . An electron in graphene has very high Fermi velocity, so motion of it is described by Dirac relativistic quantum mechanics and electrons are termed as Dirac fermions. If we calculate the effective mass of the electron, we give the following expression:

$$m^* = \hbar^2 \left(\frac{\partial^2 E}{\partial k^2}\right)^{-1}.$$
 [1.1.3]

Using the above energy dispersion relationship, we find that  $m^*$  is zero. This is another peculiar property of graphene in that it shows a "Klein Paradox".

## 1.2 Klein Paradox for spin-0 particle



Figure 1.1: A particle of energy  $E < V_0$  incident upon potential step.

The Klein Paradox [5] deals with the scattering of a particle from a potential step of a strong potential  $V_0 > E + mc^2$ . After scattering from such a strong potential, the transmission coefficient is negative and reflection coefficient is greater than one. The accepted interpretation is that, for such a strong potential, particle-antiparticle pairs are created and these created particles add to the reflected beam and so we obtain R > 1. But A.K.Geim and Novoselov resolved the Klein Paradox experimentally and proved that R can never be greater than 1, rather it can be equal to zero and  $\tau = 1$  [6] when Klein tunneling takes place. They received the Nobel Prize for this work as well as for the fabrication of graphene.

## 1.3 Organization of the Dissertation

The organization of this dissertation is as follows: In chapter 1, we describe the so called Klein Paradox and its resolution by A.K. Geim and Novoselov. In chapter 2, we briefly present features of the graphene and nanotubes, and theories to progress the dissertation. Chapter 3 gives the detailed theory about Green's function and Feynman diagrams to understand transport phenomena. Chapter 4 gives the detailed theory about relativistic quantum mechanics and Dirac plane wave solution to understand "Klein tunneling." Chapter 5 gives the detailed theory of Landauer-Buttiker formalism to progress the dissertation work. In chapter 6, we discuss Higgs mechanism that deals with the gain of mass by the particle after an interaction with Higgs field. Finally, analysis of results is presented in chapter 7. In chapter 8, conclusions and applications are included. In chapter 9, we gave appendices A and B which contain the detailed steps of the calculations and some useful theoretical aspects of Landauer-Buttiker formalism and codes used to plot graphs. At the end in chapter 10, we listed the presentations, publications and the references used in this work.

# 2 Chapter

# 2.1 Theoretical background

### 2.1.1 Introduction of the graphene sheet

Graphite is a three dimensional (3D) layered hexagonal lattice of carbon atoms. A single layer of graphite forms a two-dimensional (2D) material, 2D graphite or a graphene layer. Even in 3D graphite, the interaction between two adjacent layers is small compared with intra-layer interactions, since the layer separation of 3.35 Å is much larger than the nearest-neighbor distance between two carbon atoms which is 1.42 Å [3]. Thus the electronic structure of 2D graphite is a first approximation of that for 3D graphite.





Figure: 2.1 Three dimensional structure of graphite [30].



Figure 2.2: Graphene lattice in realFigure 2.3: Brillouin zones ofreciprocalspace with basis vectors  $\vec{a}_1$  and  $\vec{a}_2$ .lattice with basis vectors  $\vec{b}_1$  and  $\vec{b}_2$ .

#### 2.1.2 Translation vectors and periodicity

The most important property of a Bravais lattice is its translational symmetry or translational periodicity. Three vectors  $\vec{a}_1, \vec{a}_2$  and  $\vec{a}_3$  correspond to elementary translations along three different directions. These vectors are the fundamental translation vectors. To have a translational symmetry, let  $\vec{r}$  be any position in the lattice and consider another position  $\vec{r'}$  which is obtained from r such that:

$$\vec{r'} = \vec{r} + n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 , \qquad [2.1.1]$$

where  $n_1$ ,  $n_2$ , and  $n_3$  are integers.

Translational symmetry requires that the lattice arrangement appear the same at  $\vec{r'}$  as at  $\vec{r}$ . The translation vector can be expressed as

$$\vec{T} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 . \qquad [2.1.2]$$

The two-dimensional graphene lattice in real space can be created by translating one unit cell defined by

$$\vec{T} = n\vec{a}_1 + m\vec{a}_2$$
, [2.1.3]

where  $\vec{a}_1$  and  $\vec{a}_2$  are called basis vectors as shown in fig 2.2 and expressed as shown below

$$\vec{a}_1 = \left(\frac{\sqrt{3}}{2}a, \frac{a}{2}\right), \quad \vec{a}_2 = \left(\frac{\sqrt{3}}{2}a, -\frac{a}{2}\right).$$

Where a = 2.46 Å is the lattice constant of two dimensional graphite.

Correspondingly the unit vectors  $\vec{b}_1$  and  $\vec{b}_2$  of the reciprocal lattice shown in figure 2.3 can be expressed as below

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

### 2.1.3 Tight-binding energy dispersion

The tight binding model, which includes one  $p_z$  orbital per carbon atom and the nearest neighbor interaction, is used to calculate the graphene band structure. In the tight binding model, a suitable wave function is constructed that satisfies Bloch's theorem [7]

$$\psi(\vec{r} + \vec{R}) = e^{i\vec{k}.\vec{R}}\psi(\vec{r}).$$
[2.1.4]

For graphene, the tight binding wave function is a weighted sum of the two sub-lattice Bloch functions [3]:

$$\psi(\vec{k},\vec{r}) = C_A \phi_A(\vec{k},\vec{r}) + C_B \phi_B(\vec{k},\vec{r}), \qquad [2.1.5]$$

where the subscripts A and B denote the two different atoms in a unit cell of the graphene and  $C_A$  and  $C_B$  are weight factors. The Bloch functions can be expressed as a linear combination of the atomic wave functions [3]

$$\Phi_{A} = \frac{1}{\sqrt{N}} \sum_{j}^{N} e^{i\vec{k}.\vec{R}_{A_{j}}} \Phi(\vec{r} - \vec{R}_{A_{j}}), \qquad [2.1.6A]$$

$$\Phi_{B} = \frac{1}{\sqrt{N}} \sum_{j}^{N} e^{i\vec{k}.\vec{R}_{B_{j}}} \Phi(\vec{r} - \vec{R}_{B_{j}}), \qquad [2.1.6B]$$

where *N* is the number of unit cells in the lattice and  $\vec{R}_A$  and  $\vec{R}_B$  are the Bravias lattice vectors which identify the positions of all types of atoms in the graphene lattice. Here  $\frac{1}{\sqrt{N}}$  serves as normalization constant for the Bloch function.

Bloch functions must satisfy Bloch's theorem stated in the equation [2.1.4]

$$\phi_A(\vec{r} + \vec{R}_{A_l}) = e^{i\vec{k}.\vec{R}_{A_l}}\phi_A(\vec{r}). \qquad [2.1.7]$$

Schrodinger eigenvalue equation is

$$H\psi = E\psi. \tag{2.1.8}$$

Inserting equation [2.1.5] into Schrodinger equation, we obtain

$$C_A H \Phi_A(\vec{k}, \vec{r}) + C_B H \Phi_B(\vec{k}, \vec{r}) = E(k) C_A \Phi_A(\vec{k}, \vec{r}) + E(k) C_B \Phi_B(\vec{k}, \vec{r}).$$

$$[2.1.9]$$

Multiplying by the complex conjugate of  $\phi_A$ , and separately by

the complex conjugate of  $\phi_B$ , we obtain

$$C_A \phi_A^* H \phi_A + C_B \phi_A^* H \phi_B = E C_A \phi_A^* \phi_A + E(k) C_B \phi_A^* \phi_B , \qquad [2.1.10]$$

$$C_A \Phi_B^* H \Phi_A + C_B \Phi_B^* H \Phi_B = E C_A \Phi_B^* \Phi_A + E(k) C_B \Phi_B^* \Phi_B , \qquad [2.2.11]$$

Integrating both equations over the entire space, we obtain

$$C_A \int \phi_A^* H \phi_A dr + C_B \int \phi_A^* H \phi_B dr = E C_A \int \phi_A^* \phi_A dr + E C_B \int \phi_A^* \phi_B dr . \qquad [2.1.12]$$

$$C_A \int \Phi_B^* H \Phi_A dr + C_B \int \Phi_B^* H \Phi_B dr = E C_A \int \Phi_B^* \Phi_A dr + E C_B \int \Phi_B^* \Phi_B dr . \qquad [2.1.13]$$

It is customary to employ the following symbolic representation

$$H_{ij} = \int \phi_i^* H \phi_j dr , \qquad S_{ij} = \int \phi_i^* \phi_j dr , \qquad [2.1.14]$$

where  $H_{ij}$  are the matrix elements of the Hamiltonian and  $S_{ij}$  are the overlap matrix elements between Bloch functions. Since the two atoms in the unit cell are identical, therefore, the overlap matrix between all type-A atoms must be same as the overlap matrix between all type-B atoms. So we have  $S_{AA} = S_{BB}$  and also  $H_{AA} = H_{BB}$ Then,

$$C_A(H_{AA} - ES_{AA}) = C_B(ES_{AB} - H_{AB}).$$
 [2.1.15]

$$C_A(H_{AB}^* - ES_{AB}^*) = C_B(ES_{AA} - H_{AA}).$$
 [2.1.16]

Now solving  $C_B$  from equation [2.1.15] and then substituting into equation [2.1.16] We obtain

$$E(k)^{\pm} = -\frac{E_0(k) + \sqrt{E_0(k)^2 - 4(S_{AA}(k)^2 - |S_{AB}(k)|^2)(H_{AA}(k)^2 - |H_{AB}(k)|^2)}}{2(S_{AA}(k)^2 - S_{AB}(k)|^2)} \quad .$$
 [2.1.17]

with

$$E_0(k) = (2H_{AA}(k)S_{AA}(k) - S_{AB}(k)H_{AB}^*(k) - H_{AB}(k)S_{AB}^*(k)).$$
 [2.1.18]

The positive and negative energy branches in equation [2.1.17] are meant for the conduction ( $\pi^*$ ) and valence ( $\pi$ )bands respectively.

#### Nearest neighbor tight binding model:

The wave function of an electron in any primitive unit cell only overlaps with the wave functions of its nearest neighbors. This means the nearest neighbors of a type-A atom in the graphene interacts with all three types-B atoms. Therefore, according to the nearest neighbor tight binding model, the  $p_z$  wave function of a type-A atom overlaps with the  $p_z$ 

wave function of its three nearest neighbors and does not overlap anymore with wave functions from atoms farther apart.

Furthermore this simplifies equation [2.1.14] considerably [3]

$$H_{AA} = \int \Phi_{A}^{*} H \Phi_{A} dr = \frac{1}{N} \sum_{j}^{N} \sum_{l}^{N} e^{-i\vec{k}.\vec{R}_{A_{j}}} e^{ik.R_{A_{l}}} \times \int \Phi^{*} \left(\vec{r} - \vec{R}_{A_{j}}\right) H \Phi\left(\vec{r} - \vec{R}_{A_{l}}\right) dr ,$$
[2.1.19]

$$H_{AA} = \frac{1}{N} \sum_{j}^{N} \sum_{l}^{N} e^{i\vec{k}.(\vec{R}_{A_{l}} - \vec{R}_{A_{j}})} E_{2p} \delta_{jl} = E_{2p} . \qquad [2.1.20]$$

Where  $\delta_{il}$  is the Kronecker delta function.

Overlap matrix can written as

$$S_{AA}(k) = \int \Phi_{A}^{*} \Phi_{A} dr = \frac{1}{N} \sum_{j}^{N} \sum_{l}^{N} e^{-i\vec{k}.\vec{R}_{A_{j}}} e^{i\vec{k}.\vec{R}_{A_{l}}} \times \int \Phi^{*} \left(\vec{r} - \vec{R}_{A_{j}}\right) \Phi\left(\vec{r} - \vec{R}_{A_{l}}\right) dr,$$
$$S_{AA}(k) = \frac{1}{N} \sum_{j}^{N} \sum_{l}^{N} e^{i\vec{k}.(\vec{R}_{A_{l}} - \vec{R}_{A_{j}})} \delta_{jl} = 1.$$
[2.1.21]

Here we taken advantage of the normalized feature of Wannier functions,

$$\int \Phi^* \left( \vec{r} - \vec{R}_{A_j} \right) \Phi \left( \vec{r} - \vec{R}_{A_l} \right) dr = 1.$$

Electron-hole symmetry: It has been observed by ab-initio dispersion in the

neighborhood of the Fermi energy that the  $\pi$  and  $\pi^*$  have similar structure, at least for energies close to the Fermi energy E<sub>F</sub>. Since electrons are the mobile charges in the  $\pi^*$ band and holes are the mobile charges in the  $\pi$  band, so this approximation is called the electron-hole symmetry. Mathematically, electron hole symmetry leads to  $S_{AB} = 0$ Therefore, we can reduce equation [2.1.17] can be further reduced to

$$E(k)^{\pm} = E_{2p} \pm \sqrt{H_{AB}(k)H_{AB}^{*}(k)}$$
 [2.1.22]

This energy dispersion relation was originally proposed by Wallace in 1947 [8]. We can further simplify the equation by setting  $E_{2p} = 0$  [3] because the reference potential is the Fermi energy and is customarily set to 0 eV.

So we can write equation [2.1.22] as [3]

$$E(k)^{\pm} = \pm \sqrt{H_{AB}(k)H_{AB}^{*}(k)} . \qquad [2.1.23]$$

The Hamiltonian matrix element  $H_{AB}(k)$  can be calculated as follows:

$$H_{AB}(k) = \int \Phi_{A}^{*} H \Phi_{B} dr = \frac{1}{N} \sum_{j}^{N} \sum_{l}^{N} e^{i\vec{k}.(\vec{R}_{A_{j}} - \vec{R}_{B_{l}})} \times \int \Phi^{*} \left(\vec{r} - \vec{R}_{A_{j}}\right) H \Phi\left(\vec{r} - \vec{R}_{B_{l}}\right) dr .$$
[2.1.24]

Each type-A atom overlaps with three nearest neighbor type-B atoms and let the nearest neighbor distances be

$$R_1 = R_{A_j} - R_{B_j}$$
,  $R_2 = R_{A_j} - R_{B_{j+1}}$ ,  $R_3 = R_{A_j} - R_{B_{j-1}}$ ,

where j, j+1, and j-1 are the indices of the primitive unit cells. Three type-B nearest neighbor atoms are located with respect to atom A in the cell j.

Therefore,

$$H_{AB}(k) = \frac{1}{N} \sum_{j}^{N} \sum_{l}^{N} e^{-i\vec{k}.\vec{R}_{m}} E_{m}, \qquad [2.1.25]$$

where  $E_m$  is the finite value obtained the integration of the nearest neighbor Wannier function. We simply set its value  $\gamma$  which is called the hopping energy. The Hamiltonian matrix element now reduces to the following terms

$$H_{AB}(k) = \gamma \left( e^{-i\vec{k}.\vec{R}_1} + e^{-i\vec{k}.\vec{R}_2} + e^{-i\vec{k}.\vec{R}_3} \right).$$
 [2.1.26]

and

$$H_{AB}(k)H_{AB}^{*}(k) = \gamma^{2} \left( e^{-i\vec{k}.\vec{R}_{1}} + e^{-i\vec{k}.\vec{R}_{2}} + e^{-i\vec{k}.\vec{R}_{3}} \right) \left( e^{i\vec{k}.\vec{R}_{1}} + e^{i\vec{k}.\vec{R}_{2}} + e^{i\vec{k}.\vec{R}_{3}} \right) =$$
  
$$\gamma^{2} \left[ 3 + e^{i\vec{k}.(\vec{R}_{1} - \vec{R}_{2})} + e^{-i\vec{k}.(\vec{R}_{1} - \vec{R}_{2})} + e^{i\vec{k}.(\vec{R}_{1} - \vec{R}_{3}) + e^{-i\vec{k}.(\vec{R}_{1} - \vec{R}_{3})}} + e^{2i\vec{k}.(\vec{R}_{2} - \vec{R}_{3})} + e^{-i\vec{k}.(\vec{R}_{2} - \vec{R}_{3})} \right]$$
  
$$[2.1.27]$$

Now using Euler's formula  $e^{ix} + e^{-ix} = 2cosx$ , we can reduce equation [2.1.27] into the following form:

$$H_{AB}(k)H_{AB}^{*}(k) = \gamma^{2} \{3 + 2\cos[\vec{k}.(\vec{R}_{1} - \vec{R}_{2})] + 2\cos[\vec{k}.(\vec{R}_{1} - \vec{R}_{3})] + 2\cos[\vec{k}.(\vec{R}_{2} - \vec{R}_{3})] \},$$
[2.1.28]

Thus,

$$H_{AB}(k)H_{AB}^{*}(k) = \gamma^{2} \left(1 + 4\cos\frac{\sqrt{3a}}{2}k_{x}\cos\frac{a}{2}k_{y} + 4\cos^{2}\frac{a}{2}k_{y}\right).$$
 [2.1.29]

Now inserting equation [2.1.29] into equation [2.1.23], we obtain

$$E(k)^{\pm} = \pm \gamma \sqrt{1 + 4\cos\frac{\sqrt{3}}{2}ak_x \cos\frac{a}{2}k_y + 4\cos^2\frac{a}{2}k_y} \quad .$$
 [2.1.30]

This formula is widely used for graphene.

#### 2.1.4 Hybridization

Carbon has four valence electrons in the outermost orbit and tends to interact with neighboring carbon atoms to produce the different types of carbon allotrope. The ground state of carbon atom is shown as below.

The ground state configuration of carbon  $C \rightarrow 1s^2 2s^2 2p^2$ 



Figure 2.4: Ground state configuration of the carbon atom.

Excited state configuration of the carbon  $C \rightarrow 1s^2 2s^1 2p^3$ 



Figure 2.5: Excited State configuration of the carbon atom.

The four valence electrons occupy the 2s and 2p orbitals as shown above. When carbon atoms come together to form a crystal, one of the 2s electrons is excited to the  $2p_z$  orbital from energy gained from neighboring nuclei, thus lowering the overall energy of the system. The mixing of atomic orbitals is known as hybridization and new orbitals so formed are called hybrid orbitals. In the case of the graphene, there is sp<sup>2</sup> hybridization and one of the unhybridized orbitals  $2p_z$  which is perpendicular to the plane of the hybrid orbitals overlaps with the corresponding  $2p_z$  orbital of another carbon atom to form a  $\pi$ bond. The hybridized orbitals form three  $\sigma$ -bonds with neighboring carbon atoms. Graphene is considered as the mother of three carbon allotropes. When graphene is wrapped into a sphere, it produces buckyball, folding into a cylinder produces nanotube and stacking several sheets of it results in graphite. Quantum mechanically the hybridization can be expressed as follows:

Angular distribution of orbitals are given by [9]

$$|2s\rangle = \frac{1}{\sqrt{4\pi}}$$
 [2.1.31A]

$$|2p_x\rangle = \frac{1}{\sqrt{2}}(Y_1^1 + Y_1^{-1}) = \sqrt{\frac{3}{4\pi}}\sin\theta\,\cos\theta\,.$$
 [2.1.31B]

$$|2p_{y}\rangle = \frac{1}{\sqrt{2}}(Y_{1}^{1} - Y_{1}^{-1}) = \sqrt{\frac{3}{4\pi}}\sin\theta\,\sin\phi\,.$$
 [2.1.31C]

$$|2p_z > = \sqrt{\frac{3}{4\pi} \cos\theta}$$
 [2.1.31D]

Now we are going to discussing sp<sup>3</sup> hybridization which takes place in the case of diamond.



Figure 2.6: sp<sup>3</sup> hybridization in carbon atom in case of Diamond.

The wave function of a hybrid orbital [9] can be expressed as below

$$\begin{split} |\psi> &= C_1 |s> + C_2 |p_X> + C_3 |p_y> + C_4 |p_z>, \\ \text{where } \sum_{i=1}^4 C_i^2 &= 1. \end{split}$$



Figure 2.7: Orientation of hybrid orbitals with carbon atom at the center in the case of Diamond.

Let the largest possible magnitude to yield maximum overlap of orbitals be along the direction (1,1,1) of cube with carbon atom at its center with the choice

$$C_2 = C_3 = C_4 = C$$
.

So the normalization condition is given by

$$C_1^2 + 3C^2 = 1$$
. [2.1.33]  
Therefore,  $= \sqrt{(1 - C_1^2)/3}$ .

The bond forming strength [9] of  $\psi(1,1,1)$  is given by

$$C_1 + 3C = C_1 + \sqrt{3(1 - C_1^2)}$$
.

The bond forming strength will be the maximum if the differentiation of the above expression is zero.

$$\frac{d}{dC_1} \Big[ C_1 + \sqrt{3(1 - C_1^2)} \Big] = 0 \; ,$$

$$|C_1| = 1/2.$$
  
 $|C| = 1/2.$ 

The wave functions of hybrid orbitals can be expressed as follows:

$$|\psi(1,1,1)\rangle = \frac{1}{2}(|s\rangle + |p_X\rangle + |p_Y\rangle + |p_Z\rangle). \qquad [2.1.34A]$$

$$|\psi(1, -1, -1)\rangle = \frac{1}{2}(|s\rangle + |p_X\rangle - |p_Y\rangle - |p_Z\rangle). \qquad [2.1.34B]$$

$$|\psi(-1,1,-1)\rangle = \frac{1}{2}(|s\rangle - |p_X\rangle + |p_Y\rangle - |p_Z\rangle). \qquad [2.1.34C]$$

$$|\psi(-1,-1,1)\rangle = \frac{1}{2}(|s\rangle - |p_X\rangle - |p_Y\rangle + |p_Z\rangle).$$
 [2.1.34D]

The condition of maximum charge cloud density [9] in the direction of (1,1,1) is given by

$$\frac{\partial \psi(1,1,1)}{\partial \theta} = \sqrt{3}(\cos\theta\cos\varphi + \cos\theta\sin\varphi - \sin\theta) = 0.$$
 [2.1.35]

and

$$\frac{\partial \psi(1,1,1)}{\partial \phi} = \sqrt{3}(-\sin\theta \sin\phi + \sin\theta \cos\phi) = 0.$$
 [2.1.36]

Solving the above equations [2.1.35] and [2.1.36], we obtain

$$\begin{array}{ccc} \theta & \Phi \\ \psi(1,1,1) & \frac{\pi}{4} & 54^{0}44' \\ \psi(1,-1,-1) & -\frac{\pi}{4} & 125^{0}16' \end{array}$$

- $\psi(-1,1,-1)$   $\frac{3\pi}{4}$  125°15'
- $\psi(-1,-1,1)$   $5\pi/4$   $54^{0}44'$

The vectors along these directions are given as below

$$\begin{split} \vec{e}_{1,\ 1,\ 1} &= \hat{\imath} + \hat{\jmath} + \hat{k} \; . & \vec{e}_{1,\ -1,\ -1} &= \hat{\imath} - \hat{\jmath} - \hat{k} \; . \\ \vec{e}_{-1,\ 1,\ 1} &= -\hat{\imath} + \hat{\jmath} - \hat{k} \; . & \vec{e}_{-1,\ -1,\ 1} &= -\hat{\imath} - \hat{\jmath} + \hat{k} \; . \end{split}$$

The angle between, say,  $\vec{e}_{1, 1, 1}$  and  $\vec{e}_{-1, -1, 1}$  is

$$\vec{e}_{1,1,1} \cdot \vec{e}_{-1,-1,1} = |\vec{e}_{1,1,1}| |\vec{e}_{-1,-1,1}| \cos\theta$$

 $cos\theta = -1/3$  ,

$$\theta = 109^0 28' \, .$$

#### 2.2.1Carbon nanotube

A carbon nanotube can be viewed as a graphene sheet rolled along its circumferential direction [10]  $\vec{C}_h = n\vec{a}_1 + m\vec{a}_2$ , [2.2.1]

where  $\vec{a}_1$  and  $\vec{a}_2$  are the basis vectors of a graphene sheet. The unrolled honeycomb lattice of the nanotube is shown in figure 9. The vector  $\overrightarrow{OB}$  points in the direction of the nanotube axis, and the direction  $\overrightarrow{OA}$  is perpendicular to the tube axis. The vectors  $\overrightarrow{OA}$  and  $\overrightarrow{OB}$  are defined as the chiral vector  $\vec{C}_h$  and the translational vector  $\vec{T}$  of a nanotube, respectively. The chiral vector  $\vec{C}_h$  can be expressed by the real space unit vectors  $\vec{a}_1$  and  $\vec{a}_2$  of the hexagonal lattice as

 $\vec{C}_h = n\vec{a}_1 + m\vec{a}_2$ . (*n*, *m* are integers  $0 \le |m| \le |n|$ )



Figure 2.8: Representation of translation and circumferential vector.

The diameter of the carbon nanotube D is given by [10]

$$D = \frac{L}{\pi} , \qquad [2.2.2]$$

where L = circumferential length of the nanotube.

$$L = |C_h| = \sqrt{C_h \cdot C_h} = a\sqrt{n^2 + m^2 + mn}.$$

$$\vec{a}_1 \cdot \vec{a}_1 = \vec{a}_2 \cdot \vec{a}_2 = a^2, \vec{a}_1 \cdot \vec{a}_2 = a^2/2.$$
[2.2.3]

There are three types of nanotubes:

a) Armchair nanotube: An armchair nanotube corresponds to the case if

n = m that is  $C_h = (n, n)$  [10]. All armchair nanotubes exhibit metallic conduction. The nanotubes which satisfy this relation (given below) are metallic in nature, otherwise semiconducting.

 $(n-m) = 3\mu$ , where  $\mu$  is an integer.



Figure 2.9: The red line represents the circumference of the armchair variety [31].

b) Zigzag nanotube: A zigzag nanotube corresponds to the case where

m = 0, so that is  $C_h = (n, 0)$  [10].

Figure 2.10: The blue line represents the circumference of the zigzag type [31].

c) Chiral nanotube: A chiral nanotube [10] corresponds to the case where

 $n \neq m$ , so that  $C_h = (n, m)$ .



Figure 2.11: The red line shows the joining method of the chiral nanotube [31].

2.2.2: The energy dispersion of the armchair nanotube:

The periodic boundary conditions that are used to get the energy eigenvalues for the armchair nanotube can be defined by wave vectors  $k_{x,q}$  in the circumferential

direction [10]

$$n\sqrt{3} k_{x,q} a = 2\pi q$$
 , (q = 1, ...., 2n). [2.2.4]

Substituting the discrete allowed values of  $k_{x,q}$  from equation [2.2.4] into

the equation [2.1.30], we obtain

$$E(k)^{\pm} = \pm \gamma \sqrt{1 \pm 4\cos\left(\frac{q\pi}{n}\right)\cos\left(\frac{ka}{2}\right) + 4\cos^{2}\left(\frac{ka}{2}\right)} \quad .$$
$$(-\pi < ka < \pi), (q = 1, \dots, 2n) \qquad [2.2.5]$$

### 2.2.3: The energy dispersion of the zigzag nanotube:

The periodic boundary condition on  $k_y$  to obtain energy eigenvalues for the zigzag nanotube are given by the condition [10]

$$nk_{y,q}a = 2\pi q$$
,  $(q = 1, ..., 2n)$ . [2.2.6]

Substituting the discrete allowed values of  $k_{y,q}$  from equation [2.2.6] into equation [2.1.30], we obtain
$$E(k)^{\pm} = \pm \gamma \sqrt{1 \pm 4\cos\left(\frac{\sqrt{3}ka}{2}\right)\cos\left(\frac{q\pi}{n}\right) + 4\cos^{2}\left(\frac{q\pi}{n}\right)} \quad .$$

$$\left(-\frac{\pi}{\sqrt{3}} < ka < \frac{\pi}{\sqrt{3}}\right) \quad , \quad (q = 1, \dots 2n).$$

$$(2.2.7)$$

## 2.2.4: The energy dispersion of the chiral nanotube:

The translational vector is given as  $\vec{T} = t_1 \vec{a}_1 + t_2 \vec{a}_2$  (with  $t_1$  and  $t_2$  integer).

Using  $\vec{C}_h \cdot \vec{T} = 0$ , we can write

$$t_1 = \frac{(2m+n)}{d_R}$$
, and  $t_2 = \frac{-(2n+m)}{d_R}$ , [2.2.8]

where  $d_R$  is the greatest common divisor of both (2m + n) and (2n + m)[10].

Also the length of the translational vector can be given by

 $|T| = \sqrt{3} \frac{L}{d_R}$ , where *L* is the circumferencial length of the nanotube . The number of hexagons per unit cell as a function of *n* and *m* can be given by the reference [10] as

$$N = \frac{|\vec{c}_h \times \vec{T}|}{|\vec{a}_1 \times \vec{a}_2|} = \frac{2(m^2 + n^2 + nm)}{d_R} = \frac{2L^2}{a^2 d_R} .$$
 [2.2.9]



Figure 2.12: The Brillouin zone of a carbon nanotube is represented by the line segment w'w which is parallel to  $K_2$ .

The Brillouin zone of a carbon nanotube is represented by the line segment W'W which is parallel to K<sub>2</sub> [10].Now using the relations as given below, we can figure out the value of  $\vec{K}_1$  and  $\vec{K}_2$ 

where  $\vec{K}_1$  and  $\vec{K}_2$  are reciprocal lattice vectors corresponding to  $\vec{C}_h$  and  $\vec{T}$  respectively.

$$\vec{C}_h \cdot \vec{K}_1 = 2\pi, \quad \vec{T} \cdot \vec{K}_1 = 0, \ \vec{C}_h \cdot \vec{K}_2 = 0, \quad \vec{T} \cdot \vec{K}_2 = 2\pi, \quad [2.2.10]$$

$$K_1 = \frac{1}{N}(-t_2b_1 + t_1b_2), \ K_2 = \frac{1}{N}(mb_1 - nb_2).$$
 [2.2.11]

In the case of a chiral nanotube, the energy dispersion relation of two dimensional graphite,  $E_{g \ 2D}(k)$  at line segments shifted from WW' by  $K_1$ 

where  $\mu = 0, ..., N - 1$  and the value of *N* is given by equation [2.2.9].

So the energy dispersion relation [10] for chiral nanotube can be given by

$$E_{\mu}(k) = E_{g \ 2D} \left( k \frac{\overline{k_2}}{|K_2|} + \mu K_1 \right).$$

$$[2.2.12]$$
where  $-\frac{\pi}{T} < k < \frac{\pi}{T}$ .

# 3 Chapter

# 3.1 Introduction of Green Function

## 3.1.1 Green function

We have seen that many-body systems consisting of strongly interacting real particles can often be described as if they were composed of weakly interacting quasi particles and collective excitations and the properties of these particles can be evaluated with the help of quantum field theoretical quantities known as "Green functions of many-body systems" or, simply, propagators. It is not the aim to describe the detailed behavior of each particle in the system, but rather the average behavior of one or two typical particles interacting with the rest of the system. The quantities, which describe this average behavior of the particles, are the one-particle propagator and two-particle propagator respectively, and physical properties may be calculated directly from them [11]. First we consider the one-particle propagator: It is defined as the probability amplitude that we add a particle into the interacting system at point  $\vec{r_1}$  at time  $t_1$  and let it move through the system colliding with the other particles for a while and later observe. The two particle propagator is the probability amplitude to put one particle at  $\vec{r_1}$ ,  $t_1$  and another at  $\vec{r_2}$ ,  $t_2$  into the system and later observe them at  $\vec{r_3}$ ,  $t_3$  and  $\vec{r_4}$ ,  $t_4$ , respectively.

### 3.1.2 Calculating propagators by Feynman diagrams:

A particle has to move from a point 1 and needs to reach at point 2[10]. On the way to point 2, it can stop off at one or two or more points A,B,C, ....,etc. The probability P (2,1) that the particle reaches point 2 is the sum of the probabilities for all the different ways it can propagate from 1 to 2 interacting with the various interacting systems. The first way possibility to propagate from point 1 to 2 is that it propagates freely without encountering at any interacting system, and let us call this probability $P_0(2,1)$ . The second option to propagate is that it goes freely from point 1 to point A and (let its probability equal  $P_0(A, 1)$ ), then it interacts at point A (let this probability equal P(A)). Then it goes freely from point A to point 2 with its probability  $P_0(2, A)$ . The third way is to propagate from point 1 to point B and then to point 2 with total probability  $P_0(B, 1)P(B)P_0(2, B)$ . In this way, it can propagate from point 1 to point 2 through different possible ways with different probabilities. The total probability to propagate from point 1 to2 is the sum of all probabilities for each way and we can write mathematically as follows below [11].

$$P(2,1) = P_0(2,1) + P_0(A,1)P(A)P_0(2,A) + P_0(B,1)P(B)P_0(2,B) + \dots + P_0(A,1)P(A)P_0(B,A)P(B)P_0(2,B) + \dots$$
[3.1.1]

Using series [3.1.1], we can draw a diagram which is given below



Figure 3.1: A particle propagates from point 1 to point 2 and interacts with different interacting systems.

Assuming for simplicity that all  $P_0(s, r)$  are equal to the same value c i.e.,

$$P_0(2,1) = P_0(2,A) = P_0(2,B) = P_0(A,B) = c$$
.

The series [3.1.1] becomes

$$P(2,1) = c + c^{2}P(A) + c^{3}P(A)^{2} + c^{4}P(A)^{3} + \cdots$$
$$= c\{1 + c P(A) + c^{2}P(A)^{2} + c^{3}P(A)^{3} + \cdots\}$$
$$P(2,1) = c \times \left(\frac{1}{1 - cP(A)}\right) = \frac{1}{c^{-1} - P(A)} .$$
[3.1.2]

This is the solution for the propagator in this case.

3.1.3 Single-particle propagator for system of many interacting particles:

We can discuss in a qualitative way how the single-particle propagator can be calculated in a system of many particles. The propagator will be the sum of the probability amplitudes that the particle propagates from  $\vec{r_1}$ ,  $t_1$  to  $\vec{r_2}$ ,  $t_2$  through a variety of possible paths. First we have the possibility of propagation without interacting with the other particles of the system. Then we include propagation with just a single interaction. The inclusion of second, third and higher-order interactions improves the approximation of the true physical propagation. We can show these interactions by Feynman diagrams.

First we show here first-order interaction by diagrams [11].



Figure 3.2: a) A particle enters the system and interacts with any one particle of the system b) At time t, the particle is at a point  $\vec{r}$  and interacts with a particle of the system which is at a point  $\vec{r}'$  and changes its place with it. c) Extra particle leaves the system at time  $t_2$ .

a) Extra particle enters system at time  $t_1$ .

- b) At time t, the particle is at point  $\vec{r}$  and interacts with a particle of the system which is at  $\vec{r}'$  and changes place with it.
- c) Extra particle leaves the system at time  $t_2$

Second order interaction [11] is shown below:



Figure 3.3: A particle enters the system in the state k and interacts with the particle of the system and finally emerges out in the same state k.

A particle enters the system in state K at time  $t_1$  and being scattered into K-q and knocking a particle out of state l into state l+q or creating a particle into state l+q and a hole in a state l. At later time, t', the particle in K-q knocks the particle of the state l+q back into the hole state l and itself scattered into state k. This is a second order process because it involves two interactions.



Similarly we have higher-order interactions, some of which are shown below [11].

Figure 3.4: 3<sup>rd</sup> order and 4<sup>th</sup> order interaction of the particle with particles of the system.

When the extra particle enters the system, more technically we use advanced and retarded Green functions. The retarded Green function has essentially been defined above as the probability amplitude that at time  $t_1$  we add a particle at point  $r_1$  to the interacting system in its ground state, then at time  $t_2$  the system will be in its ground state with an added particle at  $\vec{r}_2$  under condition  $t_2 > t_1$ , and is denoted by  $G^+$ . Similarly, the advanced Green function ( $G^-$ ) can be defined as the probability amplitude that at time  $t_2$  we remove a particle at  $\vec{r}_2$  from the interacting system in its ground state and at time  $t_1$ , we add a particle at  $\vec{r}_1$  such that the system will be in its ground state again under condition

 $t_2 > t_1$ . This is also known as a hole propagator. Let us consider first there is free propagation from  $t_1$  to  $t_M$  in the state  $\phi_{K_1}$  and has amplitude  $G_0^+(k_1, t_M - t_1)$ . The amplitude for the second process where particle scattered from

 $\phi_{K_1}$  to  $\phi_{K_2}$  by  $V_M$  scattering potential at time  $t_M$ , which can be calculated from ordinary time-dependent perturbation theory as follows. Let  $c_l$  be the probability amplitude that at time  $t_0$  a system is in the state  $\phi_l$ . Later time t, the time rate of change of any particular state  $c_l$ , say  $c_p$ , under the perturbing potential V, can be given by

$$\dot{c}_p(t) = -i\sum_l V_{pl}c_l e^{i(\epsilon_p - \epsilon_l)(t - t_0)},$$
[3.1.3]

where  $V_{pl}$  is the matrix element of *V* between states  $\phi_p$ ,  $\phi_l$ . The probability amplitude per unit time that the system under a transition from  $\phi_{K_1}$  to  $\phi_p = \phi_{K_2}$  at time  $t = t_M$  can be given by

$$\dot{c}_{k_2} = -iV_{M_{k_2k_1}} = -i\int d^3r \phi_{k_2}^*(r) V_M \phi_{k_1}(r).$$
[3.1.4]

The amplitude for the last process is  $iG_0^+(k_2, t_2 - t_M)$ . Hence the total amplitude can be given by

$$[Probability Amplitude]_{t_{1} \to t_{M} \to t_{2}} = i \int_{-\infty}^{\infty} dt_{M} G_{0}^{+}(k_{1}, t_{M} - t_{1}) V_{M_{k_{2}k_{1}}} G_{0}^{+}(k_{2}, t_{2} - t_{M}).$$

$$[3.1.5]$$

There are second and higher-order processes in which the particle collides with large number of perturbing potentials like  $V_M$  and  $V_L$ , then the total probability amplitude can be given following expression.

Dyson's equation is given as follows:

$$G^{+}(k, t_{2} - t_{1}) = G^{+}_{0}(k, t_{2} - t_{1}) + \int_{-\infty}^{\infty} dt_{M} G^{+}_{0}(k, t_{M} - t_{1}) V_{M_{kk}} G^{+}_{0}(k, t_{2} - t_{M}) + \int_{-\infty}^{\infty} dt_{M} dt_{L} G^{+}_{0} V_{L_{kk}} G^{+}_{0} V_{M_{kk}} G^{+}_{0} + \cdots$$
[3.1.6]

Taking the Fourier transform of the above equation, we obtain

$$G^{+}(k,w) = G_{0}^{+} + [G_{0}^{+}]^{2} V_{M_{kk}} + [G_{0}^{+}]^{3} V_{M_{kk}}^{2} + \cdots$$
$$= G_{0}^{+} [1 + G_{0}^{+} V_{M_{kk}} + (G_{0}^{+})^{2} V_{M_{kk}}^{2} + \cdots]$$
$$= \frac{G_{0}^{+}}{1 - G_{0}^{+} V_{M_{kk}}} = \frac{1}{(G_{0}^{+})^{-1} - V_{M_{kk}}} \quad \text{for } |G_{0}^{+} V_{M_{kk}}| < 1.$$
[3.1.7]

The single particle Green function can also be defined as [11]

$$G(k_2, k_1, t_2 - t_1) = -i < \psi_0 | T\{c_{k_2}(t_2)c_{k_1}^{\dagger}(t_1)\} | \psi_0 >, \qquad [3.1.8]$$

where the operators  $c_k(t)$  and  $c_k^{\dagger}(t)$  respectively destroy and create a particle

in state k, at time t. We can further defined as

$$c_{k_1}^{\dagger}(t_1) = e^{iHt_1} c_{k_1}^{\dagger}(0) e^{-iHt_1}.$$
[3.1.9]

$$c_{k_2}^{\dagger}(t_2) = e^{iHt_2}c_{k_2}^{\dagger}(0) e^{-iHt_2}$$
 [3.1.10]

Also T is the time ordering operator which can be defined as

$$T\{c_{k_2}(t_2)c_{k_1}^{\dagger}(t_1)\} = c_{k_2}(t_2)c_{k_1}^{\dagger}(t_1), \text{ for } t_2 > t_1.$$
$$= -c_{k_1}^{\dagger}(t_1)c_{k_2}(t_2) \text{ for } t_2 \le t_1.$$
[3.1.11]

The time transformed Green's function is given by

$$G(E) = \sum_{i} \frac{\phi_{i}(E)\phi_{i}^{\dagger}(E)}{E - E_{i}(E)},$$
[3.1.12]

where  $\phi_i(E)$  and  $E_i(E)$  are the solutions of the energy dependent Eigen problem

$$[H^{0} + \sum(E)]\phi_{i}(E) = E_{i}(E)\phi_{i}(E). \qquad [3.1.13]$$

Here  $H^0 = K+U$  consists of kinetic energy and potential energy term and  $\sum(E)$  is the so called self-energy term. Poles of G(E) give excitation energies of the form  $E^{N\pm 1,j} - E^{N,0}$ . The first order reduced density matrix can be obtained as [12]

$$\gamma^{N,0} = \frac{1}{2\pi i} \int G(E) dz .$$
 [3.1.14]

$$E^{N,0} = \frac{1}{2\pi i} \frac{Tr}{2} \int (K + U + z) G(z) dz . \qquad [3.1.15]$$

The one body Green's function can be separated into  $\sigma$  and  $\pi$  parts. So, we can

write the one-particle Green's function as follows:

$$G(E) = G_{\sigma}(E) + G_{\pi}(E).$$
 [3.1.16]

$$G_{\pi}(E) = \frac{1}{[E - \{H^0 + \sum(E)\}]_{\pi\pi}} .$$
 [3.1.17]

$$E_{\pi}(\sigma) = \frac{1}{2\pi i} \frac{Tr}{2} \int (K + U + z) G_{\pi}(z) dz . \qquad [3.1.18]$$

Thus the total energy can be computed as

$$E^{\text{total}} = E_{\sigma}(\pi) + E_{\pi}(\sigma).$$
 [3.1.19]

# 4 Chapter

## 4.1 Application of relativistic quantum mechanics

In non-relativistic quantum mechanics, particle paths are more likely to be found in low potential regions, as there are propagating waves in the regions where the particle energy is greater than the potential energy and evanescent waves in regions otherwise. Also transmission probability exponentially depends upon potential barrier width. But in the case of relativistic quantum mechanics, massless Dirac fermions freely penetrate potential barriers of arbitrary strength with a transmission probability one for normal incidence, which is known as the Klein Paradox. Klein tunneling enables particles to tunnel through even higher potential regions that depends upon the energy of the particle, wave vector, potential profile and other parameters as well.

## 4.1.1 The Klein-Gordon equation

The Schrödinger equation in operator form is

$$\widehat{H}\psi = i\hbar\partial\psi/\partial t . \qquad [4.1.1]$$

But now in the relativistic case, we have the energy momentum relation for a free particle

$$E^2 = c^2 p^2 + m^2 c^4. ag{4.1.2}$$

Replacing *E* and *p* by the corresponding operators  $i\hbar \frac{\partial}{\partial t}$  and  $-i\hbar\nabla$ , we obtain the Klein-Gordon equation for free particle [13] as follows:

$$\frac{1}{c^2}\frac{\partial^2 \Phi}{\partial t^2} - \nabla^2 \Phi + \frac{m^2 c^2}{\hbar^2} \Phi = 0. \qquad [4.1.3]$$

This is the Klein-Gordon equation for free particles.

## 4.1.2 Charge and current density

Taking the complex conjugate of above equation [4.1.3], we obtain

$$\nabla^2 \Phi^* - \frac{1}{c^2} \frac{\partial^2 \Phi^*}{\partial t^2} - \frac{m^2 c^2}{\hbar^2} \Phi^* = 0.$$

$$[4.1.4]$$

Multiplying equations [4.1.3] and [4.1.4] by  $\phi^*$  and  $\phi$  respectively, we obtain

$$\Phi^* \nabla^2 \Phi - \frac{1}{c^2} \Phi^* \frac{\partial^2 \Phi}{\partial t^2} - \frac{m^2 c^2}{\hbar^2} \Phi^* \Phi = 0.$$
[4.1.5]

and

$$\Phi \nabla^2 \Phi^* - \frac{1}{c^2} \Phi \ \frac{\partial^2 \Phi^*}{\partial t^2} - \ \frac{m^2 c^2}{\hbar^2} \Phi \Phi^* = 0 \ . \tag{4.1.6}$$

Subtracting equation [4.1.6] from equation [4.1.5], we obtain

$$\Phi^* \nabla^2 \Phi - \Phi \nabla^2 \Phi^* - \frac{1}{c^2} \left( \Phi^* \frac{\partial^2 \Phi}{\partial t^2} - \Phi \frac{\partial^2 \Phi^*}{\partial t^2} \right) = 0,$$

which can be written as

$$\vec{\nabla} \cdot \left[ \Phi^* \vec{\nabla} \Phi - \Phi \vec{\nabla} \Phi^* \right] - \frac{1}{c^2} \frac{\partial}{\partial t} \left[ \Phi^* \frac{\partial \Phi}{\partial t} - \frac{\partial \Phi^*}{\partial t} \Phi \right] = 0.$$

$$[4.1.7]$$

Multiplying equation [4.1.7] by  $\frac{\hbar}{2im}$ , we obtain

$$\vec{\nabla} \cdot \left[\frac{\hbar}{2im} (\phi^* \vec{\nabla} \phi - \phi \vec{\nabla} \phi^*)\right] + \frac{\partial}{\partial t} \left[\frac{\hbar}{2imc^2} (\phi^* \frac{\partial \phi}{\partial t} - \frac{\partial \phi^*}{\partial t} \phi)\right] = 0,$$

or

$$\vec{\nabla} \cdot \vec{j} + \frac{\partial \rho}{\partial t} = 0.$$
[4.1.8]

where probability current density is given as follows:

$$\vec{j} = \frac{\hbar}{2im} (\phi^* \vec{\nabla} \phi - \phi \vec{\nabla} \phi^*).$$
[4.1.9]

The probability density is

$$\rho = \frac{\hbar}{2imc^2} \left( \Phi^* \frac{\partial \Phi}{\partial t} - \frac{\partial \Phi^*}{\partial t} \Phi \right).$$
[4.1.10]

### 4.2.1 Dirac's relativistic equation

The Klein-Gordon equation is a second-order equation in time and one could specify both  $\phi$  and  $\frac{\partial \phi}{\partial t}$  separately at a given time. The problem is that the probability density  $\rho$  may take on both positive and negative values since the energy of a free particle is given by

$$E = \pm \sqrt{c^2 p^2 + m^2 c^4} \,. \tag{4.2.1}$$

Hence  $\rho$  cannot be interpreted as a probability density. Therefore, Dirac formulated a relativistic wave equation which avoids the difficulty arising from the Klein-Gordon equation by working directly with the square root as an operator and linearized the energy expression [14] as follows

$$\sqrt{\sum_{i=1}^{3} p_i^2 + m^2 c^2} = \sum_{i=1}^{3} \alpha_i p_i + \beta m c , \qquad [4.2.2]$$

where  $\alpha_1, \alpha_2, \alpha_3$ , and  $\beta$  are some non-commutative operators which are specified through their algebraic properties.

In order that the right-hand side of equation [4.2.2] is equivalent to the left side of it. It is necessary that

$$(\sum_{i=1}^{3} \alpha_i p_i + \beta mc)(\sum_{k=1}^{3} \alpha_k p_k + \beta mc) = p_1^2 + p_2^2 + p_3^2 + m^2 c^2, \qquad [4.2.3]$$

$$\alpha_1^2 p_1^2 + \alpha_2^2 p_2^2 + \alpha_3^2 p_3^2 + \alpha_3^2 m_0^2 c^2 + (\alpha_1 \alpha_2 + \alpha_2 \alpha_1) p_1 p_2 + \dots + \dots + (\alpha_1 \beta + \beta \alpha_1) p_1 m_0 c + \dots + \dots = p_1^2 + p_2^2 + p_3^2 + m^2 c^2 .$$

$$[4.2.4]$$

Equating both sides, we find the algebraic properties

$$\alpha_1^2 = \alpha_2^2 = \alpha_3^2 = \beta^2 = 1.$$
 [4.2.5]

$$\alpha_i \alpha_k + \alpha_k \alpha_i = 0. \quad i, k = 1, 2, 3 \quad for \ i \neq k$$

$$[4.2.6]$$

$$\alpha_i \beta + \beta \alpha_i = 0$$
. where  $i = 1, 2, 3$  [4.2.7]

### 4.2.2 Dirac Matrices

The squares of any of the four matrices are unity and their eigen-values are +1 and -1.

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} .$$
 [4.2.8]

In terms of the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

$$[4.2.9]$$

Dirac's matrices are given by

$$\alpha_x = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix} , \ \alpha_y = \begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix} , \ \alpha_z = \begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix}.$$
 [4.2.10]

Substituting the right hand side of equation [4.2.2] into equation [4.2.1], we obtain the linearized energy equation

$$E - c \sum_{i=1}^{3} \alpha_i p_i - \beta m_0 c^2 = 0. \qquad [4.2.11]$$

In terms of the energy and momentum operators, we write Dirac's equation in the following form

$$\left(i\hbar\frac{\partial}{\partial t} + ci\hbar\sum_{k=1}^{3}\alpha_{k}\frac{\partial}{\partial x_{k}} - \beta m_{0}c^{2}\right)\psi(x,t) = 0.$$

$$[4.2.12]$$

## 4.2.3 The Dirac equation

The Dirac equation can be given by

$$(c\vec{\alpha}\cdot\vec{p}+\beta mc^2)\psi = E\psi \qquad [4.2.13]$$

or 
$$(c\alpha_x p_x + c\alpha_y p_y + c\alpha_z p_z + \beta mc^2)\psi = E\psi$$
.

In a more explicit form, we replace  $\alpha's$  and  $\beta$  by specific matrices and replacing  $\psi$  by a four-component symbol

$$\begin{pmatrix} mc^{2} & 0 & cp_{z} & c(p_{x}-ip_{y}) \\ 0 & mc^{2} & c(p_{x}+ip_{y}) & -cp_{z} \\ cp_{z} & c(p_{x}-ip_{y}) & -mc^{2} & 0 \\ c(p_{x}+ip_{y}) & -cp_{z} & 0 & -mc^{2} \end{pmatrix} \begin{pmatrix} \psi_{1} \\ \psi_{2} \\ \psi_{3} \\ \psi_{4} \end{pmatrix} = E \begin{pmatrix} \psi_{1} \\ \psi_{2} \\ \psi_{3} \\ \psi_{4} \end{pmatrix}.$$
[4.2.14]

This equation is equivalent to the four simultaneous equations

$$(E - mc^{2})\psi_{1} + i\hbar c \frac{\partial\psi_{3}}{\partial z} + i\hbar c (\frac{\partial}{\partial x} - i\frac{\partial}{\partial y})\psi_{4} = 0.$$
[4.2.15A]

$$(E - mc^2)\psi_2 + i\hbar c \left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)\psi_3 - i\hbar c \frac{\partial\psi_4}{\partial z} = 0.$$
 [4.2.15B]

$$(E - mc^{2})\psi_{3} + i\hbar c \frac{\partial\psi_{1}}{\partial z} + i\hbar c (\frac{\partial}{\partial x} - i\frac{\partial}{\partial y})\psi_{2} = 0.$$
 [4.2.15C]

$$(E - mc^2)\psi_4 + i\hbar c \left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)\psi_1 - i\hbar c \frac{\partial\psi_2}{\partial z} = 0.$$
 [4.2.15D]

## 4.2.4 Free particle or plane wave solution of Dirac's equation

The wave function  $\psi$  has four components and the Dirac equation is exactly a set of four first order linear partial differential equations. The plane wave solution [13] can be represented as follows,

$$\psi_j(r,t) = u_j e^{i(\vec{k}.\vec{r}-wt)}.$$
[4.2.16]

where = 1, 2, 3, 4.

After substituting in the equation [4.2.15A], [4.2.15B], [4.2.15C] and [4.2.15D], we obtain

$$(E - mc2)u_1 - cp_z u_3 - c(p_x - ip_y)u_4 = 0.$$
 [4.2.17A]

$$(E - mc2)u_2 - c(p_x + ip_y)u_3 - cp_z u_4 = 0.$$
 [4.2.17B]

$$(E + mc2)u_3 - cp_z u_1 - c(p_x - ip_y)u_2 = 0.$$
 [4.2.17C]

$$(E + mc2)u_4 - c(p_x + ip_y)u_1 + cp_z u_2 = 0.$$
 [4.2.17D]

These equations are homogeneous and have non trivial solution only if the determinant of the matrix is zero,

$$\begin{vmatrix} (E - mc^2) & 0 & -cp_z & -c(p_x - ip_y) \\ 0 & (E - mc^2) & -c(p_x + ip_y) & cp_z \\ -cp_z & -c(p_x - ip_y) & (E + mc^2) & 0 \\ -c(p_x + ip_y) & cp_z & 0 & (E + mc^2) \end{vmatrix} = 0,$$
  
or  $(E^2 - c^2 p^2 - m^2 c^4)^2 = 0.$  [4.2.18]

This is in agreement with energy-momentum relation for a free particle.

From equation [4.2.18], we obtain

$$E = \pm \sqrt{c^2 p^2 + m^2 c^4} \,. \tag{4.2.19}$$

Taking first positive energy solution  $E_+ = +\sqrt{c^2p^2 + m^2c^4}$ .

There are two linearly independent solutions which can be written from last of two equations [4.2.17]

$$u_1 = 1$$
 ,  $u_2 = 0$  ,  $u_3 = \frac{cp_z}{E_+ + mc^2}$  ,  $u_4 = \frac{c(p_x + ip_y)}{E_+ + mc^2}$  . [4.2.20A]

$$u_1 = 0$$
 ,  $u_2 = 1$  ,  $u_3 = \frac{c(p_x - ip_y)}{E_+ + mc^2}$  ,  $u_4 = \frac{-cp_z}{E_+ + mc^2}$  . [4.2.20B]

Similarly, from the negative energy solution  $E_{-} = -\sqrt{c^2 p^2 + m^2 c^4}$ .

we obtain two new solutions from the first two of equations [4.2.17]

$$u_1 = \frac{cp_z}{E_- - mc^2}$$
,  $u_2 = \frac{c(p_x + ip_y)}{E_- - mc^2}$ ,  $u_3 = 1$ ,  $u_4 = 0$ . [4.2.21A]

$$u_1 = \frac{c(p_x - ip_y)}{E_- - mc^2}$$
,  $u_2 = \frac{-cp_z}{E_- - mc^2}$ ,  $u_3 = 0$ ,  $u_4 = 1$ . [4.2.21B]

Each of these solutions can be normalized by multiplying it by a factor N so that

 $\psi^* \psi = 1$ or,  $N^2 [u_1^* u_1 + u_2^* u_2 + u_3^* u_3 + u_4^* u_4] = 1$ or,  $N^2 \left[ 1 + 0 + \frac{c^2 p^2}{(E_+ + mc^2)^2} + \frac{c^2 (p_x^2 + p_y^2)}{(E_+ + mc^2)^2} \right] = 1$  $N = \left[ 1 + \frac{c^2 p^2}{(E_+ + mc^2)^2} \right]^{-1/2}.$  [4.2.22]

4.2.5 Probability density and current density

The Dirac equation for a free particle [13] is

$$i\hbar\frac{\partial\psi}{\partial t} + i\hbar c \,\vec{\alpha} \cdot \vec{\nabla} \,\psi - \beta m c^2 \psi = 0. \qquad [4.2.23]$$

Taking the Hermitian conjugate of equation [4.2.23], we obtain

$$-i\hbar\frac{\partial\psi^{\dagger}}{\partial t} - i\hbar c \,\nabla\psi^{\dagger} \cdot \vec{\alpha} - \psi^{\dagger}\beta mc^{2} = 0. \qquad [4.2.24]$$

Multiplying equation [4.2.23] on the left by  $\psi^{\dagger}$  and equation [4.2.24] on the right

side by  $\psi$ 

$$i\hbar\psi^{\dagger}\frac{\partial\psi}{\partial t} + i\hbar c\,\psi^{\dagger}\,\vec{\alpha}\cdot\vec{\nabla}\,\psi - mc^{2}\psi^{\dagger}\beta\psi = 0. \qquad [4.2.25]$$

$$-i\hbar\frac{\partial\psi^{\dagger}}{\partial t}\psi - i\hbar c \,\nabla\psi^{\dagger}\cdot\vec{\alpha}\psi - mc^{2}\psi^{\dagger}\beta\psi = 0. \qquad [4.2.26]$$

Subtracting equation [4.2.26] from equation [4.2.25], we obtain

$$i\hbar\frac{\partial}{\partial t}(\psi^{\dagger}\psi) + i\hbar \ c \ \nabla. (\psi^{\dagger}\alpha\psi) = 0.$$
[4.2.27]

We can thus identify the probability charge density and current density from above equation [4.2.27] as follows:

$$\rho = \psi^{\dagger} \psi \,. \tag{4.2.28}$$

$$j = c \psi^{\dagger} \alpha \psi \,. \tag{4.2.29}$$

## 4.3.1 The Klein paradox for spin-0 particle



Figure 4.1: A particle of energy  $E < V_0$  which is incident upon a finite potential barrier.

Consider a particle of energy E and momentum p. Let c = 1 and  $\hbar = 1$ 

$$V(Z) = 0$$
  $Z < 0$ .  
=  $V_0$   $Z > 0$ . [4.3.1]

The Klein-Gordon equation in the presence of this potential is [5]

$$\partial_t^2 \phi_{<} - \nabla^2 \phi_{<} + m^2 \phi_{<} = 0$$
 for  $Z < 0.$  [4.3.2]

$$(i\partial_t - V_0)^2 \phi_{>} + \nabla^2 \phi_{>} - m^2 \phi_{>} = 0 \quad \text{for } Z > 0.$$
 [4.3.3]

The solutions of the Klein –Gordon equation are

$$\Phi_{<} = e^{-iEt} \left[ e^{ipz} + r e^{-ipz} \right], \qquad [4.3.4]$$

$$\Phi_{>} = t \, e^{-iEt} \, e^{ip'z} \,, \tag{4.3.5}$$

where r and t are the reflection and the transmission amplitude, respectively and p' is momentum of the particle inside potential step.

Substituting these solutions into the Klein-Gordon equation, we obtain

$$E^2 - p^2 - m^2 = 0$$
 for  $Z < 0$   
or  $E = \pm \sqrt{p^2 + m^2}$  for  $Z < 0$ . [4.3.6]

$$E^{2} + V_{0}^{2} - 2EV_{0} - p'^{2} - m^{2} = 0 \quad \text{for } Z > 0$$
  
or  $p' = \pm \sqrt{(E - V_{0})^{2} - m^{2}} \quad \text{for } Z > 0.$  [4.3.7]

#### **Case I: Weak Potential**

$$V_0 < E - m \rightarrow (E - V_0) > m$$

Then p' is real.

#### **Case II: Intermediate Potential**

$$(E-m) < V_0 < (E+m) \rightarrow |E-V_0| < m$$

Then, p' is imaginary.

#### **Case III: Strong potential**

$$V_0 > (E+m) \rightarrow |E-V_0| > m$$

Then p' is real.

Now imposing the boundary condition that  $\phi$  and  $\partial_Z \phi$  be continuous at Z = 0

$$e^{-iEt}(1+r) = te^{-iEt}$$
 [4.3.8]

$$e^{-iEt}ip(1-r) = ip'te^{-iEt}$$
. [4.3.9]

Solving equations [4.3.8] and [4.3.9] we obtain

$$1 + r = t$$
. [4.3.10]

$$1 - r = p't/p$$
. [4.3.11]

Again solving these equations, we obtain

$$t = \frac{2p}{p+p'}$$
 and  $r = \frac{(p-p')}{(p+p')}$ . [4.3.12]

We know that the probability current density is defined as

$$\vec{j} = \frac{1}{2im} \left[ \phi^* \vec{\nabla} \phi - \phi \vec{\nabla} \phi^* \right].$$
[4.3.13]

The incident probability current density is

$$j_I = p/m.$$
 [4.3.14]

Similarly, the probability current density for regions Z > 0 and Z < 0 can be obtained by using the equation [4.3.13]

$$j_{>} = \frac{(p'+p'^{*})|t|^{2}}{2m} e^{i(p'-p'^{*})z} = \frac{p'|t|^{2}}{m} . \quad \text{for real } p' \qquad [4.3.15]$$

= 0. for imaginary p'

$$j_{<} = \frac{p}{m} \left( 1 - |r|^{2} \right).$$
[4.3.16]

Now we can define the transmission co-efficient as

$$\tau = \frac{j_{>}}{j_{I}} = \frac{(p'+p'^{*})|t|^{2}}{2p} e^{i(p'-p'^{*})z} = \frac{2p(p'+p'^{*})}{(p+p')(p+p'^{*})} e^{i(p'-p'^{*})z}.$$
 [4.3.17]

Similarly the reflection co-efficient R =  $1 - |\tau| = |\frac{(p-p')}{p+p'}|^2$ . [4.3.18]

#### **Case I: Weak Potential**

p' is real and transmission co-efficient and reflection co-efficient can be given as

$$\tau = \frac{4pp'}{(p+p')^2}$$
 and  $R = \left(\frac{p-p'}{p+p'}\right)^2$ .

So, we have  $\tau + R = 1$  non relativistic matching.

#### **Case II: Intermediate Potential**

$$p' = \text{imaginary}$$
  
 $\tau = 0 \text{ and } R = 1.$ 

So, again we have  $\tau + R = 1$  non relativistic matching.

#### **Case III: Strong Potential**

Taking *p*'real and negative  $\tau = -\frac{4p|p'|}{(p-|p'|)^2}$  and  $R = \left(\frac{p+p'}{p-p'}\right)^2 > 1$ .

Hence R > 1 and  $\tau = -Ve$  relativistic matching. Therefore, the reflection coefficient is greater than one and transmission coefficient is negative. This surprising result is called the Klein Paradox.

## 4.3.2 The Klein Paradox for spin-1/2 particle

The Dirac Hamiltonian can be given by the following expression [14]

$$H = \vec{\alpha} \cdot \vec{p} + \beta m, \qquad [4.3.19]$$

where we use the standard choice of  $c = \hbar = 1$ .

The eigenvalues of the Hamiltonian are

$$E = \pm \sqrt{p^2 + m^2} \,. \tag{4.3.20}$$

For positive energy solutions of  $spin \pm 1/2$ , the spinors can be introduced as

$$u_{+} = \begin{pmatrix} 1\\ 0\\ 0\\ 0 \end{pmatrix} \quad \text{and} \ u_{-} = \begin{pmatrix} 0\\ 1\\ 0\\ 0 \end{pmatrix}.$$
 [4.3.21]

For negative energy solutions of  $spin\pm 1/2$ , the spinors can be expressed as

$$v_{+} = \begin{pmatrix} 0\\ 0\\ 1\\ 0 \end{pmatrix}$$
 and  $v_{-} = \begin{pmatrix} 0\\ 0\\ 0\\ 1 \end{pmatrix}$ . [4.3.22]

Alternately, we can write the eigenvalue equation in terms of two component spinors

 $u_1$  ,  $u_2$  ,  $v_1$  and  $v_2$ 

$$u_{\pm} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$$
 and  $v_{\pm} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$ . [4.3.23]

$$\left[\vec{\alpha}\cdot\vec{p}+\beta m\right]\binom{u_1}{u_2}=E\binom{u_1}{u_2}.$$
[4.3.24]

Substituting the matrices  $\alpha$  and  $\beta$  in the equation [4.3.24], we obtain

$$mu_1 + \vec{\sigma} \cdot \vec{p} \, u_2 = E(p)u_1,$$
 [4.3.25]

$$-mu_2 + \vec{\sigma} \cdot \vec{p} \, u_1 = E(p)u_2, \qquad [4.3.26]$$

Solving these equations yields

$$u_2 = \frac{(\vec{\sigma} \cdot \vec{p})u_1}{[E(p)+m]}.$$
 [4.3.27]

Now we can write the spinors as

$$u_{\pm} = \sqrt{\frac{E(p) + m}{2m}} \binom{u_1}{\binom{(\vec{\sigma} \cdot \vec{p})u_1}{[E(p) + m]}}.$$
 [4.3.28]

Similarly we can express other spinor as

$$v_{\pm} = \sqrt{\frac{E(p) + m}{2m}} \binom{v_1}{\left(\frac{(\vec{\sigma} \cdot \vec{p})v_1}{[E(p) + m]}\right)}.$$
 [4.3.29]

we can write the incident, reflected and transmitted waves as follows:

$$\psi_I = \begin{pmatrix} 1 \\ 0 \\ \frac{p}{E+m} \\ 0 \end{pmatrix} e^{i\vec{p}\cdot\vec{z}} , \quad \psi_R = r \begin{pmatrix} 1 \\ 0 \\ \frac{-p}{E+m} \\ 0 \end{pmatrix} e^{-i\vec{p}\cdot\vec{z}} \text{ and } \psi_T = t \begin{pmatrix} 1 \\ 0 \\ \frac{p'}{E'+m} \\ 0 \end{pmatrix} e^{i\vec{p}\vec{r}\cdot\vec{z}} ,$$

where r and t are reflection and transmission amplitudes, respectively.

Waves are continuous. So applying the boundary condition at Z = 0, we obtain

$$\begin{pmatrix} 1\\0\\\frac{p}{E+m}\\0 \end{pmatrix} + r \begin{pmatrix} 1\\0\\\frac{-p}{E+m}\\0 \end{pmatrix} = t \begin{pmatrix} 1\\0\\\frac{p'}{E'+m}\\0 \end{pmatrix}.$$
[4.3.30]

Equating the coefficients on both sides, we obtain

$$1 + r = t,$$
 [4.3.31]

and

$$\frac{p}{E+m}(1-r) = t \frac{p'}{E'+m}$$
or  $1-r = \frac{p'(E+m)t}{p(E'+m)}$ 
or,  $1-r = \xi t$ 

$$[4.3.32]$$
where  $= \frac{p'(E+m)}{p(E'+m)}$ .

Solving equations [4.3.31] and [4.3.32], we obtain

$$t = \frac{2}{1+\xi}$$
 and  $r = 1 - \xi t = 1 - 2\xi/(1+\xi)$ . [4.3.33]

The probability current density is given by  $J_I = \psi^{\dagger} \alpha \psi = \psi^{\dagger} \begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix} \psi$ 

$$= \begin{pmatrix} 1 & 0 & \frac{p}{E+m} & 0 \end{pmatrix} \begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ \frac{p}{E+m} \\ 0 \end{pmatrix} = \frac{2p}{(E+m)}$$
[4.3.34]

Similarly, we can write the probability current density for transmitted and reflected waves as

$$J_T = \frac{(p'+pr^*)|t|^2}{(E'+m)}$$
 and  $J_R = \frac{-2p|r|^2}{(E+m)}$ . [4.3.35]

The transmission coefficient can be given as follows:

$$\tau = \frac{j_T}{j_I} = \frac{\frac{(p'+p^{*})|t|^2}{(E'+m)}}{2p/(E+m)} = \frac{2(\xi+\xi^*)}{|1+\xi|^2} .$$
[4.3.36]

and the reflection coefficient is given by

$$R = -|\frac{1-\xi}{1+\xi}|^2 > 1.$$
 [4.3.37]

This result is called the Klein Paradox. It found its experimental refutation in the work of K. S. Novoselov and A. K. Geim [6]. The general idea of the experiment is shown in the figure 4.2 where the potential barrier has rectangular shape and is infinite along the y-axis.



Figure 4.2: A particle of energy  $E < V_0$  tunnels through barrier width D.

$$V(x) = \begin{cases} V_0 \ 0 < x < D \\ 0 & \text{otherwise.} \end{cases}$$
[4.3.38]

Because of experimental requirements, it is arranged that the incident electron wave propagates at a small angle  $\phi$  with respect to the *x* axis, and the components of the Dirac spinor  $\psi_1$  and  $\psi_2$  for the Hamiltonian  $H = H_0 + V(x)$  in the following form [6]:

$$\begin{pmatrix} (e^{ik_x x} + re^{-ik_x x})e^{ik_y y} & x < 0. \\ (e^{ik_x x} + re^{-ik_x x})e^{ik_y y} & x < 0. \end{cases}$$

$$[4.3.39A]$$

$$\psi_1 = \begin{cases} (ae^{iq_x x} + be^{-iq_x x})e^{ik_y y} & 0 < x < D. \end{cases}$$

$$[4.3.39B]$$

$$(te^{ik_x x + ik_y y} \qquad x > D. \qquad [4.3.39C]$$

$$(s(e^{ik_x x} - re^{-ik_x x - i\phi})e^{ik_y y} x < 0.$$
 [4.3.40*A*]

$$\psi_2 = \left\{ \left( a e^{i q_x x - i\theta} - b e^{-i q_x x - i\theta} \right) e^{i k_y y} \quad 0 < x < D. \right.$$

$$[4.3.40B]$$

$$(ste^{ik_x x + ik_y y + i\phi} \qquad x > D.$$

$$[4.3.40C]$$

With  $k_F = \frac{2\pi}{\lambda}$  as the Fermi wave number. We can express  $k_x = k_F cos \phi$  and

 $k_y = k_F sin \Phi$  as the wave vector components outside the barrier. Inside the barrier we have the momentum which is given below

$$q_x = \sqrt{\frac{(E-V_0)^2}{\hbar^2 v_F^2} - k_y^2}$$
,  $\theta = \tan^{-1}\left(\frac{k_y}{q_x}\right)$  is the refraction angle.

$$s = \operatorname{sgn} E$$
 and  $s' = \operatorname{sgn}(E - V_0)$ .

Using the continuity of the wave function by matching coefficients b, t and r we obtain the following equation for the reflection coefficient [6]

$$r = 2ie^{i\Phi}sin(q_x D) \frac{sin\Phi - ssysin\theta}{ss'[e^{-iq_x D}\cos(\Phi + \theta) + e^{iq_x D}\cos(\Phi - \theta)] - 2isin(q_x D)} \quad [4.3.41]$$

Transmission probability can be given by the following expression as shown below

$$T = 1 - |r|^2 . [4.3.42]$$

Using this expression we can find the expression for the angular dependence of the transmission probability in the limit of high barrier  $V_0 \gg |E|$ 

$$T = \frac{\cos^2 \Phi}{1 - \cos^2(q_x D) \sin^2 \Phi} \quad [4.3.43]$$

Using above expressions reflection and transmission coefficient under resonance conditions  $q_x D = \pi N$ ,  $N = 0, \pm 1, ...$  the barrier becomes transparent at normal incidence  $\phi = 0$ 

i.e. 
$$T = 1$$
 and  $R = 0$ . [4.3.44]



Figure 4.3: Transmission probability T through a 100nm wide barrier as function of the incident angle for graphene with electron concentration n outside the barrier is chosen as  $0.5 \times 10^{12} \text{ cm}^{-2}$  and inside barrier , hole concentrations p are  $1 \times 10^{12}$  and  $3 \times 10^{12} \text{ cm}^{-2}$ .

# 5 Chapter

## 5.1 Theory of Transport Phenomena

### 5.1.1 Landauer-Buttiker formalism

The phase coherence length of electrons in mesoscopic systems, like graphene, nanotubes, fullerenes etc., can be several microns long. As a consequence, electronic transport properties of small mesoscopic devices will completely rely on quantum coherence effects. So in a mesoscopic system, quantum transport phenomena are usually described by the Landauer-Buttiker approach. To understand this approach, we need to know some common physical quantities described below.

#### 5.2.1 Fermi level and Fermi energy

The Fermi-Dirac function f(E) gives the probability that a single particle state of energy *E* is occupied by an electron [16]

$$f(E) = \frac{1}{1+e^{\left[\frac{E-\mu}{k_BT}\right]}},$$
 [5.2.1]

where  $\mu$  is the chemical potential and  $k_B$  and T are the Boltzmann's constant and the absolute temperature, respectively. At absolute zero, for  $E > E_F(\text{ or } \mu)$  it must be f(E) = 0 and for  $E \le E_F$ , f(E) = 1 as all levels are occupied. Therefore, the probability of finding an electron on a level with energy  $E > E_F$  is zero and the probability of finding an electron with energy  $E \le E_F$  is 1.



Figure 5.1: Graph of the Fermi function vs. energy a) at absolute temperature T = 0 and b) at absolute temperature T > 0.

The Fermi level is defined as the highest occupied quantum level in the valence band at zero Kelvin in the case of a metal. But for semiconductors and insulators, it is located in the band gap of valence and conduction bands. At higher temperatures a certain fraction, characterized by the Fermi function, occupies levels above the Fermi level. In doped semiconductors, the Fermi level shifts from the middle position. Fermions obey the Pauli Exclusion Principle, i.e. no two fermions can be in the same quantum state. To determine the lowest energy of a system of fermions, we add particles to unoccupied states with the lowest energy and thus fill the particles up to the Fermi level. When all the particles have been put in, the energy of the highest occupied state is called Fermi energy.



Figure 5.2: Graph of energy vs. Fermi-distribution function a) at absolute temperature

T = 0 and b) at absolute temperature T > 0.

In the case of a one dimensional infinite square well of length L, the energy of the nth state can be given by the following expression:

$$E_n = \frac{\hbar^2 \pi^2}{2mL^2} n^2, \qquad [5.2.2]$$

where *n* is the *n*th quantum state.

Suppose we have N particles in the system. The energy of the 1<sup>st</sup> quantum state is given by

$$E_1 = \frac{\hbar^2 \pi^2}{2mL^2}.$$
 [5.2.3]

This value of energy is occupied by two particles of spin, up and down. Similarly in the next quantum state, particles have the energy  $E_2 = \frac{4 \hbar^2 \pi^2}{2mL^2} = 4E_1$  and so forth.

In this way energy levels up to n = N/2 are occupied and all higher levels are empty. The Fermi energy is therefore given by the following expression given below

$$E_F = E_{N/2} = \frac{\hbar^2 \pi^2}{2mL^2} (N/2)^2 \qquad [5.2.4]$$

In the case of the three dimensional cubical box of length L, the single particle energies are given by

$$E_{n_{x,n_{y,n_{z}}}} = \frac{\hbar^{2}\pi^{2}}{2mL^{2}} \left( n_{x}^{2} + n_{y}^{2} + n_{z}^{2} \right), \qquad [5.2.5]$$

where  $n_x$ ,  $n_y$  and  $n_z$  are positive integers. Now introducing  $n_F^2 = n_x^2 + n_y^2 + n_z^2$ . Then each quantum state corresponds to a point in n-space with energy

$$E_n = \frac{\hbar^2 \pi^2}{2mL^2} n_F^2 \qquad [5.2.6]$$

The number of states with energy less than  $E_F$  is equal to the number of states that lie within a sphere of radius n in the n-space. In the ground state, this number equals the number of fermions in the system which is

$$N = 2 \times \frac{1}{8} \times \frac{4}{3} \pi n_F^3 \,. \tag{5.2.7}$$

The factor 2 for two spin states and the factor 1/8 because only 1/8 of the sphere lies in the region where all n are positive.

So the Fermi energy is given as follows:

$$E_n = \frac{\hbar^2 \pi^2}{2mL^2} n_F^2 = \frac{\hbar^2 \pi^2}{2mL^2} \left(\frac{3N}{\pi}\right)^{2/3}$$

Therefore,

$$E_n = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V}\right)^{2/3} .$$
 [5.2.8]

#### 5.3.1 Density of states

Many physical phenomena depend on the number of the quantum states within a certain energy range. When a semiconducting device absorbs light, electrons can jump from occupied valence states to unoccupied states. The energy of the photons must match the energy difference between occupied and unoccupied states. The probability of transition depends on the number of unoccupied states available. So, the transition probability depends critically on the density of states available in the valence and conduction bands. The density of states is defined as the number of energy states per unit energy range per unit volume of the device.

Density of states = 
$$g(E) = \frac{\text{number of states}}{\text{energy} \times \text{volume}}$$
.


Figure 5.3: Schematic graph of energy vs. number of states.

Suppose we have a system with discrete energy levels and the device has a volume of say  $1 \text{ cm}^3$ . The figure shows that the number of states is 4 in the energy interval between 3eV and 4 eV. So the density of states at energy E = 3 eV must be given as follows:

$$g(3) = \frac{\text{number of states}}{\text{Energy} \times \text{volume}} \frac{4}{1 \text{eV} \times 1 \text{cm}^3} = 4.$$

Generally, we use finer energy scales if the material has a large numbers of states, then we represent the density of states in K-space. <u>Density of states in 3-dimensions</u>: There is one allowed value of K per volume  $\left(\frac{2\pi}{L}\right)^3$  in

*K*-space. So the number of states in the volume  $\frac{4}{3}\pi K^3$  can be given as below [18]

The number of states *N* in the volume  $\frac{4}{3}\pi K^3 = \left(\frac{L}{2\pi}\right)^3 \times \frac{4}{3}\pi K^3$ 

$$\frac{dN}{dK} = \frac{VK^2}{2\pi^2}$$

$$D(\omega) = g(\omega) = \frac{dN}{d\omega} = \frac{dN}{dK} \frac{dK}{d\omega} = \frac{VK^2}{2\pi^2} \frac{dK}{d\omega}$$
$$D(\epsilon) = \frac{dN}{d\epsilon} = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \epsilon^{1/2}.$$
 [5.3.1]

where we have used  $\epsilon = \frac{\hbar^2 K^2}{2m}$ .

# Case 1 : 2-dimensional graphene:

The number of states *N* in the area  $\pi K^2 = \left(\frac{L}{2\pi}\right)^2 \pi K^2$ .

In the case of graphene the energy of the particle is  $\epsilon = \hbar K v$  in the relativistic limit [6]

where v is the velocity of the electron inside graphene.

So, the number of states *N* in the area  $\pi K^2 = \left(\frac{L}{2\pi}\right)^2 \pi \frac{\epsilon^2}{\hbar^2 v^2}$ 

Therefore,

The density of states [6] per unit area is evaluated as  $(\epsilon) = \frac{dN}{d\epsilon} = \frac{|\epsilon|}{2\pi\hbar^2 v^2}$ . [5.3.2]

# Case 2: 1-dimensional nanotubes:

The number of states in the length  $K = \frac{L}{2\pi}K = \frac{L}{2\pi}\frac{\epsilon}{\hbar\nu}$ .

Therefore,

Density of states per unit length 
$$(E) = \frac{dN}{d\epsilon} = \frac{1}{2\pi\hbar\nu}$$
. [5.3.3]

# 5.4.1 Transmission function

Consider a particle of energy, E, approaching a potential barrier of height  $U_0>E$  from the left. According to quantum mechanics, the probability that the particle penetrates the potential barrier is not zero as in classical mechanics. Thus the transmission coefficient is the probability that the particle penetrates the barrier and exits at point a.



Figure 5.4: A particle of energy  $E < U_0$  incident upon barrier of width a

In our case, we determine the transmission coefficient as follows: Consider a linear channel with a repulsive potential  $U(z) = U_0 \delta(z)$  at z = 0.



Figure 5.5: A particle of energy  $E < V_0$  tunnels through barrier.

Let wave function of the incident wave be  $\psi_I = e^{ikz}$  and the reflected wave function  $\psi_R = re^{-ikz}$  where *r* is the reflection amplitude. Now the transmitted wave function can be represented as  $\psi_T = te^{ikz}$ , where *t* is the transmission amplitude.

The wave functions are continuous at z = 0

So, 
$$1 + r = t$$
. [5.4.1]

Also, the derivative of the wave function is discontinuous at z = 0

$$\left[\frac{d\psi}{dz}\right]_{z=0^+} - \left[\frac{d\psi}{dz}\right]_{z=0^-} = \frac{2mU_0}{\hbar^2} \left[\psi\right]_{z=0} , \qquad [5.4.2]$$

or 
$$ik[t - (1 - r)] = \frac{2mU_0t}{\hbar^2}$$

Solving equations [5.4.1] and [5.4.2], we obtain

$$t = \frac{ik\hbar^2}{ik\hbar^2 - mU_0} \ .$$
 [5.4.3]

Now using  $p = \hbar k$  and  $\frac{p}{m} = v$ , we obtain

$$t = \frac{i\hbar\nu}{i\hbar\nu - U_0} \ . \tag{5.4.4}$$

Transmission coefficient [17] (E) = Trace  $[\Gamma_1 G \Gamma_2 G^{\dagger}] = |t|^2 = \frac{\hbar^2 v(E)^2}{\hbar^2 v(E)^2 + U_0^2}$ . [5.4.5]

(More explanation is given in Appendix A)



5.4.2 What makes electrons to move from source to drain?

Figure 5.6: Transmission of electron from source to Drain.

Conduction depends on the availability of states around chemical potential irrespective of whether states are empty or filled. To understand the mechanism of the conduction of electrons from the source to the drain, we have shown figure 5.6. When the source is connected to the negative electrode of the battery and the drain connected to the positive electrode of the battery, the chemical potential of the source increases but the drain decreases with respect to the chemical potential of the channel, thus maintaining them at a distinct chemical potential difference equal to the product of the electronic charge and the potential difference of the battery. This difference of the chemical potential between the source and drain causes electrons to flow from the source to the drain

$$\mu_1 - \mu_2 = eV . [5.4.6]$$

The contact of the source and the drain with the battery gives rise to different Fermi functions which are given below

$$f_1(E) = \frac{1}{1 + exp((E - \mu_1)/K_B T)} = f_0(E - \mu_1).$$
 [5.4.7]

$$f_2(E) = \frac{1}{1 + exp((E - \mu_2)/K_B T)} = f_0(E - \mu_2).$$
 [5.4.8]

The current in the circuit can be given by the following expression as shown below

$$I(E) = \frac{e^{T(E)}}{\pi\hbar} [f(E - \mu_1) - f(E - \mu_2)].$$
 [5.4.9]

This is the Landauer-Buttiker formula [17].

where, T(E) is the transmission function which is given by the formula

$$T(E) = Tr[\Gamma_1(E)G^R(E)\Gamma_2(E)G^A(E).$$
[5.4.10]

At zero temperature the Fermi function becomes the Heaviside step function  $\theta(\mu_j - E)$ .

Therefore,

$$I(E) = \frac{MeT(E)}{\pi\hbar} [\Theta(E - \mu_S) - \Theta(E - \mu_D)] dE = \frac{2e^2M}{\hbar} TV.$$
 [5.4.11]

where M is the number of modes or channels.

# 6 Chapter

# 6.1 Theory of gaining mass of an electron in graphene

## 6.1.1 Higgs Mechanism

The mechanism in which particles gain mass by interacting with the Higgs field is called the Higgs mechanism, first introduced by Peter Higgs [18]. The Higgs boson is associated with a field, called the Higgs field, which pervades the universe everywhere. Every force is associated with some type of a particle. The particle of electromagnetism is the photon, a massless boson. The weak force is associated with particles called W and Z bosons which are very massive, and it is believed that this mass is brought about through the Higgs mechanism. Higgs boson has been searched for since 1970 and on July 4<sup>th</sup>, 2012, CERN announced the likely discovery of a Higgs field and thereby are supposed to gain mass. Heavier particles interact more with the Higgs field and gain more mass, whereas particles of zero mass do not interact with the Higgs field and therefore remain massless. The electron in graphene is massless but gains mass when the graphene is folded into a nanotube. There are two common explanations of the gaining of mass:

- i) Through the Higgs Mechanism
- ii) Through compactification of space dimensions

#### 6.1.2 Theory of the Higgs Mechanism

After a review of the shortcomings of the electroweak interaction in the Standard Model, the gauge fields are introduced to the local gauge invariance of the particle field. The Lagrangian density describing gauge-invariance forbids a mass term for Higgs bosons. Consider the Lagrangian density [19] for a real scalar Klein-Gordon field  $\Phi$ ,

$$L = T - V = \frac{1}{2} (\partial_l \Phi) (\partial^l \Phi) - V(\Phi), \text{ With } V(\Phi) = -\frac{1}{2} \mu^2 \Phi^2 + \frac{1}{4} \lambda^2 \Phi^4 .$$
 [6.1.1]

The potential  $V(\Phi)$  is a function of the generalized coordinate  $\Phi(x)$  and has a parabolic shape around the minimum at  $\Phi(x) = 0$ . This Lagrangian exhibits simple reflection symmetry under  $\Phi = -\Phi$  about the minimum. If  $\mu^2 > 0$  the minimum of potential corresponds to  $\Phi(x) = 0$ 

If, however,  $\mu^2 < 0$ , we find the minimum of the potential by setting

$$\frac{\partial V}{\partial \phi} = 0 \rightarrow \Phi(\mu^2 + \lambda \Phi^2) = 0.$$

The choice  $\Phi(x) = 0$  is not a minimum of the potential. The potential will be minimal at

$$\Phi = \pm \sqrt{\frac{\mu^2}{\lambda}} \equiv v.$$
 [6.1.2]

To determine the particle spectrum, we added a small perturbation such that

$$\Phi(x) = v + \eta(x)$$

Under this condition, the Lagrangian density is

$$L = \frac{1}{2} (\partial_{l} \Phi) (\partial^{l} \Phi) + \frac{1}{2} \mu^{2} \Phi^{2} - \frac{1}{4} \lambda^{2} \Phi^{4} = \frac{1}{2} (\partial_{l} (\Phi + \eta) (\partial^{l} (\Phi + \eta)) + \frac{1}{2} \mu^{2} (\Phi + \eta)^{2} - \frac{1}{4} \lambda^{2} (\Phi + \eta)^{4}$$

$$= \frac{1}{2} (\partial_{l} \eta) (\partial^{l} \eta) + \frac{1}{2} \mu^{2} \eta^{2} + \mu^{2} v \eta + \frac{1}{2} \mu^{2} v^{2} - \frac{1}{4} \frac{\mu^{2}}{v^{2}} (\eta^{4} + v^{4} + 4\eta^{3} v + 4\eta v^{3} + 6\eta^{2} v^{2})$$

$$= \frac{1}{2} (\partial_{l} \eta) (\partial^{l} \eta) - \mu^{2} \eta^{2} - \frac{1}{4} \frac{\mu^{2}}{v^{2}} (\eta^{4} + 4\eta^{3} v) + \frac{1}{4} \eta^{2} v^{2}.$$
[6.1.3]
Kinetic energy Term mass term higher order term constant

Due to the Higgs field  $\eta$ , the symmetry is broken and this leads to the mass term. This is called spontaneous symmetry breaking.



Graph of Potential vs. phi with  $\mu = \pm 20$  and  $\lambda = 4$ 

Figure 6.1: The graph of potential of the Higgs field vs. field Phi.



Figure 6.2: a) Two highly accelerated electron beams interact with other and thereby there is a creation of Z- boson as well as Higgs boson b) Higgs boson immediately annihilates into two photons.

We obtained a kinetic Klein-Gordon term for field  $\eta$ , a proper mass term and a triple and quartic vertex coupling terms of the field  $\eta$ .



Figure 6.3: Photo of CERN Lab where Higgs boson was believed to be found where 2,600 employees and 8000 scientists and engineers are working.

## 6.1.3 Compactification of space dimension

In graphene, near Dirac points, the effective mass of electrons and holes approach zero. This leads to a propagation speed of  $10^6$  m/s. But the electrons and holes acquire some mass when graphene is folded into a nanotube. According to A.D. Alhaidari [20], the effective mass generation comes naturally from rolling up a graphene sheet into a tube simply by changing the space topology from 2D to 1D. So there is an existence of extra space like dimensions with an electron in graphene. The effective mass can be given by the relation

$$m = \left| \mu \right| / R , \qquad [6.1.4]$$

where  $\mu$  is constant and *R* is the radius of the tube .

For graphene, the radius of curvature is

$$R = \infty.$$
[6.1.5]

Therefore, the effective mass of the electron is zero.

# 7 Chapter

#### 7.1 Results and discussion

# 7.1.1 The graph of energy vs. wave vector for graphene

Why do we apply relativistic quantum mechanics here? First, there are many experimental phenomena which cannot be explained using purely non-relativistic quantum mechanics. Second, it would be profoundly unsatisfactory if relativity and quantum mechanics could not be united. Finally, one would expect new phenomena when a particle attains almost relativistic velocity inside nano-materials like graphene and nanotubes. When a free particle enters a region where there is an external potential, which paths will the particle follow [21]? Classically, the possible paths are strictly confined to the regions where the energy of the particle is greater than its potential energy. Accordingly, in non-relativistic quantum mechanics, particle paths are more likely to be found in low potential regions, as there are propagating waves in the regions where the particle energy is greater than the potential energy [21], and the transmission probability depends exponentially upon potential strength. But in the case of relativistic quantum mechanics, massless Dirac fermions freely penetrate potential barriers of arbitrary strength with transmission probability one for normal incidence, which is known as the Klein Paradox.

Klein tunneling enables particles to tunnel through higher potential regions. This process depends upon the energy of the particle, its wave vector, the potential profile and other parameters as well. In transport through graphene, the electrons follow paths associated with high potential rather than those with low potential, and this anomalous behavior of the flow of the particles leads to extreme conductance fluctuations.

Carbon atoms in graphene are arranged on a honeycomb lattice, and this unique configuration of the structure leads to an unusual energy dispersion relation near the Brillouin zone corners.

As shown in figures 7.1 and 7.2, the valence (E < 0) and conduction (E > 0) bands nearly touch at six pairs of points in the Brillouin zone corners, of which two sets of points are inequivalent. These two points in reciprocal lattice (K and K') are known as Dirac points where the Hamiltonian is given by the following expression [21]

$$\widehat{H} = \pm i\hbar v_F \vec{\sigma} \cdot \vec{\nabla}, \qquad [7.1.1]$$

where  $\sigma = (\sigma_x, \sigma_y)$  are Pauli matrices and  $v_F = 10^6 m/s$  is the Fermi velocity in graphene. The + (-) sign corresponds to taking the approximation near the K (K') points, and electrons near these Dirac points move with the Fermi velocity  $v_F = 10^6 m/s$ .



Figure 7.1: Graph of energy vs.  $ak_x$  and  $ak_y$  in graphene where "a" is lattice constant and  $k_x$  and  $k_y$  are wave vectors along the x and y directions, respectively. Golden color and violet color show conduction bands and valence bands, respectively.

Now the above graph of energy vs. wave vectors is rotated to indicate the Dirac points where the effective mass of an electron is zero. The two sets of Dirac points are shown inside the red circle.



Energy vs. wave

Figure 7.2: The graph shows two sets of Dirac points where the effective mass of the electron is zero.

7.1.2 Transmission through graphene and its density of states and band structure

When an electron moves through a graphene lattice, it gains a virtual spin known as pseudospin. Quasiparticles in graphene are chiral, meaning that the orientation of the electron's pseudospin is either parallel or antiparallel to the direction of its momentum, and this property remains conserved inside of graphene.



Figure 7.3 (a): Two counter-propagating particles creating a phase difference of  $\pi$ .



Figure 32 (b): Conservation of chirality of the particles in graphene.

As electrons propagate around closed paths, the pseudospin remains parallel to the momentum as shown in the figure above. For a clockwise path, the pseudospin rotates by an angle of  $-\pi$  in the graphene plane and for an anticlockwise path, the angle of pseudospin rotates by  $\pi$ . The difference in the pseudospin for the counter-propagating paths is then  $2\pi$ . Analogous to the rotation of a spin-1/2 fermion, for which a rotation by  $2\pi$  doesn't return the wave function to its original state, a net rotation of the pseudospin by  $2\pi$  induces a phase difference of  $\pi$  between the counter-propagating paths [23] and causes destructive interference and suppresses the backscattering of particles. So, the transmission inside graphene is unique. Now we can show the nature of the unique transmission of particles inside graphene.



Figure 7.4: A two dimensional graphene sheet in between two electrodes through which the transmission spectrum has been calculated [32].



Figure 7.5: Graph of energy vs. transmission coefficient of graphene as obtained with the Atomistix Toolkit Package [32].

Here, we can see that the nature of the transmission is not uniform everywhere in the region of -2 eV to +2 eV. In the region around 0 eV the transmission coefficient is small, but beyond in the negative region of energy, it is of increasing nature and reaches its maximum and then decreases until around -1 eV. In the region of -1 eV, the transmission remains low and fluctuates until around -1.4 eV and then increases and reaches its maximum, and then it decreases to around 0.26 because the trend of the density of states

is increasing and reaches a maximum, then decreases beyond -1.4 eV. The value of the transmission coefficient may be greater than one if the number of channels is greater than one. In the positive region of the energy, the value of the transmission is fluctuating until 1eV, and afterward its value increases because the trend of the density of state increases, which is shown in figure 7.5. The transmission is not the same in positive and negative regions of the energy because the coupling of the channel to the source and drain is not the same. The transmission function critically depends on the density of states of the channel. The density of the states of graphene is shown below.



Figure 7.6: Graph of the density of states vs. energy of graphene obtained with the Atomistix Toolkit Package [32].

In the negative region from 0 to -1 eV, the density of states is fluctuating, but beyond that its value increases sharply and then decreases around -2 eV. In the positive region of the energy, the density of states increases up to 2 eV. So, the nature of the density of states is different in positive and negative regions and depends on the band structure of the channel. The band structure of graphene is shown below.



Figure 7.7: Band structure of graphene as obtained with the Atomistix Toolkit [32].

In this case, the energies have the values  $\pm 3t$ ,  $\pm t$  and 0, respectively, at the high symmetry points  $\Gamma$ , K, and M in the Brillouin zone. Thus the band width gives |6t|, which is consistent with the three connected  $\pi$  bonds. The  $\pi$  and the two  $\sigma$  bands have different symmetries, and so do the  $\pi^*$  and the two  $\sigma^*$  bands. The nature of the current through the channel depends on the corresponding band structure and the transmission function.



Figure 7.8: Current-voltage characteristics of graphene as obtained with the Atomistix Toolkit package [32].

The current is fluctuating in the region from 0.5 eV to around 1.5 eV and then increases. In the negative region of the bias voltage from -0.5 eV to -1.5 eV, the current fluctuates little and then increases. In both positive bias and negative bias, it shows negative differential resistance (NDR) which plays a very important role in electronic devices.

Again, the high temperature normalized electrical resistance [24] can be theoretically approximated as [24]



Figure 7.9: The graph of the normalized resistance vs. temperature for graphene.

Also, the transmission probability T (E) depends only weakly on the barrier height, approaching perfect transparency for very high barriers. In equation [4.3.43], we have for the present case the momentum  $q_x = \sqrt{\frac{(E-V_0)^2}{\hbar^2 v_F^2} - k_y^2}$ .



Figure 7.10: Graph of transmission vs. barrier height (meV) for graphene.

We see that the transmission probability depends also only weakly on the barrier width as shown below:



Figure 7.11: Transmission coefficient vs. barrier width (nm) of graphene.

Here it looks as if the transmission coefficient remains constant at the angle of incidence  $phi=1^{0}$  but by changing the range of the scale, we can see that it depends weakly on the barrier width which is shown below:



Figure 7.12: Transmission coefficient vs. barrier width (nm) at phi =  $1^{0}$  for the case of graphene.

Again we see a weak dependence of the transmission function on the barrier width at phi equal to  $30^{0}$ .



Transmission probability vs. barrier width with phi=  $30^{\circ}$  and B.H. = 450meV

Figure 7.13: Transmission coefficient vs. barrier width (nm) at  $phi = 30^{\circ}$  for graphene.

# 7.2.1 Transmission through nanotubes of different diameters and their band structure

The structure of carbon nanotubes has been explored by transmission electron microscopy (TEM) and scanning tunneling microscopy (STM), and it has been found that they are cylinders derived from the honeycomb lattice of a monolayer of the graphite sheet [10]. The single walled nanotubes are characterized as having strong covalent bonds, exceptionally high tensile strength, high resilience as well as electronic properties ranging from semiconducting to metallic and high thermal capacity. The most fundamental property of nanotubes is their electrical conductivity. The ballistic conduction has been verified for a single carbon nanotube over the length of 200 nm [24] at room temperature, as well as at low temperatures. [25], [26]. Due to these peculiar properties of nanotubes, transistors made of nanotubes and graphene are 10 to 100 times faster than our silicon based transistors. We calculated the energy per atom for graphene and nanotubes using the DFT program. Since the energy per atom in the cases of graphene and nanotubes are different, band structures, density of states and transmission coefficients are different also. The speed of an electron in graphene is  $1.1 \times 10^6 m/s$ , and in a nanotube its value is  $1.0 \times 10^6 m/s$ . Therefore, we have studied the transport properties through nanotubes of different diameters. The transmission curves through nanotubes of different diameters are different. In the case of a nanotube with a diameter of 4.383 nm, the transmission coefficient shows a decreasing trend in the positive bias and an increasing trend in the negative bias. But in the case of a nanotube with a diameter of 3.1629 nm, the transmission curve shows an increasing trend in the positive bias, and

an initially decreasing trend and then increasing trend in the negative bias. Similarly, in the case of a nanotube with a diameter of 2.4388 nm, the transmission coefficient shows an increasing trend initially and then decreasing trend in the positive bias, whereas its value shows an increasing trend in the negative bias.

7.2.2 Transmission through nanotubes of diameter 4.383 nm and its band structure

Nanotube of diameter 4.3830 nm: It has been found that nanotubes of different diameters have different bond lengths and different energies per atom. The nanotubes of larger diameters have smaller bond lengths and possess less energy per atom [33]. As band structures of different diameter nanotubes are different, transmission properties tend to differ. The nanotube with a diameter of 4.3830 nm has a bond length of 1.428 Å. (see fig.7.14).



Figure 7.14: Nanotubes of diameter 4.3830 nm through which the transmission spectrum has been calculated with the Atomistix Toolkit Package [32].



Figure 7.15: Graph of the transmission coefficient vs. energy for a nanotube of diameter 4.383nm [32].

The transmission spectra in the positive as well as negative energy regions are not the same. The transmission coefficient beyond 0 eV is fluctuating and shows a decreasing trend in the positive region because of the decreasing trend of density of states in those regions. In the negative regions, the transmission coefficient is a fluctuating but

increasing trend. The value of the transmission coefficient is larger at -2 eV than +2 eV. Beyond -1.0 eV, the average values of the transmission coefficient are higher than the average values beyond +1.0 eV. This is caused by the density of states which is different in these regions. The density of states as a function of energy is given below



Figure 7.16: Graph of the density of states vs. energy for a nanotube of diameter 4.383 nm with Atomistix Toolkit Package [32].

The density of states is rapidly fluctuating from 0 eV to 2 eV. In negative voltage regions, the density of states is also fluctuating but has much higher values beyond -1 eV.



Figure 7.17: Band structure of a nanotube of diameter 4.383 nm with the Atomistix

Toolkit Package [32].

Due to the curvature effect, we encounter  $\pi^* - \sigma^*$  hybridization and the  $\pi^* - \sigma^*$  states mix and repel each other, resulting in a lowering of the energy as compared to the original  $\pi^*$  states. This drastically changes the electronic band structure from that obtained by simply folding the graphite sheet band structure [28]. Thus, allowed wave vectors are different than graphene, and the transmission of current through a nanotube is different than through a graphene sheet.



Figure 7.18: The graph of current vs. voltage in the nanotube of diameter 4.383 nm as obtained with Atomistix Toolkit Package [32].

The current in the positive bias voltage and negative bias voltage is not symmetric because of asymmetry of the band structure. In the positive bias voltages, current fluctuates more, and in the negative bias voltage, it fluctuates less. Its value is maximum around -1.8 eV and then decreases.

7.2.3 Transmission through nanotube of diameter 3.6129 nm and its band structure

Nanotube of diameter 3.6129 nm: This nanotube has a bond length of 1.430 nm and has approximately 0.063 eV more energy per atom than the nanotube of diameter 4.383 nm [33]. So its transmission property is different from the previous one. The system of the nanotube attached with electrodes is shown below.



Figure 7.19: The nanotube of diameter 3.6129 nm for which the transmission spectrum has been calculated with Atomistix Toolkit Package [32].



Figure 7.20: Graph of the transmission coefficient vs. energy for a nanotube of diameter 3.6129 nm as obtained with Atomistix Toolkit Package [32].

The transmission in the positive region as well as the negative region is not symmetric. Beyond 1eV, the transmission coefficient highly fluctuates and then decreases because of similar trend of density of states in those regions. In the negative voltage regions, the trend of the transmission coefficient is also fluctuating and reaches to around 3.75eV and
then decreases because of the similar trend found in density of states in those regions.

This is caused by an asymmetry of the corresponding density of states.



Figure 7.21: Density of states vs. energy for a nanotube of diameter 3.6129nm as obtained with Atomistix Toolkit Package [32].

The transmission is not symmetric in positive and negative regions because the density of states fluctuates differently in the two regions. It increases up to approximately 20/ev in the negative region but reaches a surprisingly high maximum value of 45/eV in the positive region.



Figure 7.22: The band structure of a nanotube of diameter 3.6129 nm with Atomistix Toolkit Package [32].

Due to curvature effect, there is a stronger  $\pi^* - \sigma^*$  hybridization and the hybridized states strongly repel each other, resulting in a lowering in the energy compared with the original  $\pi^*$  states. This drastically changes the electronic band structure from the nanotube of diameter 4.383nm. So, the transmission is different from a nanotube of diameter 4.383nm, and this causes a difference in current.



Figure 7.23: The graph of current vs. voltage for a nanotube of diameter 3.6129 nm as obtained with Atomistix Toolkit Package [32].

The current in both positive and negative regions of bias voltage is again not symmetric because of asymmetry of the transmission. In the positive region, we find a stronger fluctuation of the current beyond 1V and reaches maximum of 68000 nA and then decreases. But in the negative region, there is less pronounced fluctuation in the current, and its value reaches around a maximum of 75000 nA and then slightly decreases.

7.2.4 Transmission through nanotubes of diameter 2.4338 nm and its band structure

Nanotube of diameter 2.4338 nm: This nanotube has a bond length of 1.445 nm and thus has approximately 0.25 eV more energy per atom than the previous nanotube [33]. The band spectrum as well as the transmission is noticeably different from the other nanotubes we studied. The system of nanotube attached with electrodes is shown below.



Figure 7.24: The nanotube of diameter 2.4338 nm for which the transmission spectrum has been calculated as obtained with Atomistix Toolkit Package [32].



Figure 7.25: Transmission coefficient vs. energy for a nanotube of diameter 2.4338 nm as obtained with Atomistix Toolkit Package [32].

The transmission through this nanotube reflects again the asymmetric nature of the density of states about the Fermi level. The transmission spectrum is highly fluctuating and has a maximum value up to 1.6 and decreases below 0.2 at 2 eV in positive regions. The values of transmission coefficients are also fluctuating in negative regions, and its

value reaches to a maximum value over 1.6 and decreases to around 0.9 at -2 eV because a similar trend of density of states is found in those regions.



Figure 7.26: Graph of density of states vs. energy for a nanotube of diameter 2.4338 nm with Atomistix Toolkit Package [32].

The values of the density of states are fluctuating in positive regions of energy with a maximum value of 55 eV<sup>-1</sup> and then decreases to around 5 eV<sup>-1</sup>, whereas in the negative regions of energy, its values fluctuate even more with a maximum of 60 eV<sup>-1</sup> and then decreases to 11 eV<sup>-1</sup>.



Figure 7.27: The band structure of nanotube having diameter 2.4338 nm as obtained with Atomistix Toolkit Package [32].

Since its surface is strongly curved, there is very strong  $\pi^* - \sigma^*$  hybridization and states strongly mix with each other which lead to repulsion, resulting in a lowering of the energy of original  $\pi^*$  states. This leads to a drastic change of the band structure compared to the nanotube of diameter 3.6129 nm. Consequently, the transmission of the two nanotubes differs noticeably.



Figure 7.28: The graph of current vs. voltage for a nanotube of diameter 2.4338 nm as obtained with Atomistix Toolkit Package [32].

The current in the positive bias and negative bias is again not symmetric because of asymmetry of the transmission. The current fluctuates slowly in the positive region of bias voltage and finally reaches to around 42000 nA, but in negative regions, current fluctuates highly and reaches to around 680000 nA.

Also, the electrical conductivity of a nanotube obeys power law [29] is given by the expression given below



$$G(T) \propto T^{\alpha}$$
, where  $\alpha = 0.3 \text{ to } 0.6$ . [7.2.1]

Figure 7.29: The graph of conductance of a nanotube vs. temperature. The red line and the blue line show conductance vs. temperature when  $\alpha = 0.3$  and 0.6, respectively.

# 7.2.5 Calculation of total electronic energies per atom by density functional theory.

Electronic energy of different molecules has been calculated by B3LYP functional which is the most popular high-level computational method in density functional theory. B3 symbolizes Becke's three-parameter hybrid functional, and LYP is a gradient-corrected correlation functional developed by Lee, Yang and Parr. 6-31G (d) basis function has been used in this calculation. Since band structure of a material much depends upon energy per atom, we calculated energy per atom of graphene, nanotube and other organic molecules which contain carbon atoms using the DFT program. Organic structural isomers are taken in order to check that energy per atom is approximately the same as graphene and nanotube or not.

Molecule	Energy(Ha)/Atom	Energy(eV)/Atom
Graphene	-38.34693163	-1043.496704
Nanotube	-38.29107055	-1041.976612
Pentacene	-38.49090651	-1047.414548
Dibenz[a, j]anthracene	-38.49210232	-1047.447088
Picene	-38.49209807	-1047.446973

Table1: Energy calculation for different molecules by density functional theory.



Figure 7.30: Structure of graphene whose electronic energy has been calculated.



Figure 7.31: Structure of nanotube whose electronic energy has been

calculated.



Figure 7.32: Structure of pentacene whose electronic energy has been calculated.



Fig. 7.33: Structure of Dibenz [a,j]anthracene whose electronic energy has been calculated.



Figure 7.34: Structure Picene whose electronic energy has been calculated.

# 8 Chapter

#### 8.1 Discussion:

We calculated the transmission of electrons through a graphene sheet and then folded the graphene sheet into a cylindrical structure which is a carbon nanotube. The energy per atom increases when the graphene sheet is bent into a nanotube, which is verified by density functional theory (DFT). Since the energy of the graphene sheet is different from that of a nanotube, the band structure, as well as the density of states differs in for both cases. For the same reason the transmission in both cases is different. We also plotted graphs of the transmission coefficient and current vs. voltage for three nanotubes of different diameters using the "Atomistix Toolkit Package". We obtained different graphs in all three cases. The value of the transmission co-efficient may be greater than one if the number of channels is greater than one. We also computed the total electronic energy of several organic compounds like pentacene, Dibenz[a,j]anthracene and Picene using density functional theory to evaluate the energy per carbon atom keeping the number of carbon atoms and hydrogen atoms the same in all three cases, and thus verifying that the energy of different structure isomers have approximately the same energy as that of the graphene and carbon nanotubes. It has been found that indeed structural isomers exhibit only slight differences in energy per atom. Similarly, we found that the energies of graphene sheets and nanotubes also differ. In other words, we suggest that the energy surplus of a nanotube adds up to whatever energy we apply to fold a graphene sheet. Therefore, graphs of transmission vs. energy, current vs. voltage, band structure and

density of states for all the studied structures differ. When electrons propagate through graphene, they interact with the lattice and thereby gain a pseudospin quantum number. The pseudospin angular momentum and the direction of linear momentum align in the same direction, which is known as chirality. Also, destructive interference takes place between clockwise and counterclockwise particle motion inside graphene because the phase difference between them is  $\pi$ . Due to chirality and destructive interference between clockwise and counter clockwise particle motion inside graphene, the reflection coefficient becomes zero and the transmission coefficient becomes one, leading to the resolution of the Klein Paradox. The effective mass of an electron in the environment of a graphene sheet is zero, but, when the graphene sheet is bent into a carbon nanotube, the electron interacts with a Higgs-like field and spontaneous breaking of the symmetry of the Higgs field takes place. This is one possible accepted explanation for the effective mass of the electron becoming non-zero. Alternatively, one has argued that a graphene sheet with its 2-dimensional topology, when it is folded into a carbon nanotube, is reduced to a 1-dimensional topology. Therefore, an electron is associated with one extra space like dimension inside a graphene sheet, but, when it is folded into a carbon nanotube, loses one of the space dimensions. Thereby, the effective mass of an electron inside the carbon nanotube becomes non-zero due to compactification of space dimensions. When we plot the graph of energy vs. wave vectors, we get a conduction band which is shown in red color and a valence band which is shown in violet color. The conduction band is characterized by E > 0 and valence band is characterized by E < 0. When this plot is rotated, we exhibit two pairs of points which are known as Dirac points.

The effective mass of the electron is zero at Dirac points and has Fermi velocity  $1.1 \times 10^6 m/s$ .

For an angle of incidence  $1^{\circ}$ , the transmission probability vs. barrier width seems to be an approximately straight line, i.e. transmission probability is independent of barrier width. When the y-range is decreased, the transmission probability seems to be very weakly dependent upon the barrier width which is shown in the figure 7.12. For an angle of incidence of  $30^{\circ}$ , the transmission probability is weakly dependent upon barrier width as shown in figure 7.13. The dependence of the transmission vs. barrier height is also plotted, and it is found that the transmission probability depends very weakly on the barrier height. We can say that there is an approximately perfect transmission of electrons through a barrier. The transmission depends also on the density of states in the case of carbon nanotubes as well as graphene and it is found that wherever the density of states is higher, the transmission is found to be higher too. In the case of graphene, the trend of the density of states beyond 1 eV is increasing and so the transmission coefficient also increases beyond 1 eV and, similarly, the density of states initially increases and decreases beyond -1.5 eV and the transmission probability also initially increases and then decreases beyond -1.5 eV. Also, we found similar dependencies of the transmission probability on the density of states in the case of carbon nanotubes. Graphene and nanotubes show negative differential resistance (NDR) behavior, i.e. the current decreases as the voltage increases. We observed that graphene and nanotubes show NDR behavior in the negative as well positive bias. Also, the current vs. voltage graphs for the cases of graphene and nanotubes are different because of curvature effect,

i.e. which is explained by hybridization between  $\pi^*$  and  $\sigma^*$  bands. These states mix and repel each other, resulting in a lowering of the energy as compared to the original nonhybridized states. This causes relevant changes in the band structure and explains the differences in the transmission in the case of graphene and carbon nanotubes. The differences of the transmission in positive and negative bias are not symmetric because of an asymmetry of the coupling of the channels with the electrodes. To calculate the energy of graphene and nanotube by density functional theory, the number of carbon atoms in both systems has been taken equal, but the number of hydrogen atoms is necessarily different. The total energy obtained is then divided by the number of atoms present in the molecule including the hydrogen atoms. In pentacene, dibenz [a,j]anthracene and Picene, the number of hydrogen atoms taken are same. We umber of atoms present in the molecule including hydrogen atoms. We found that every structural isomer has very little difference of energy.

#### 8.2 Applications of graphene and nanotubes

Graphene and carbon nanotubes show negative differential resistance (NDR) behavior which is characterized by a decreasing current with an increasing bias voltage. The property of NDR behavior has become the basic principle of several electronic devices such as resonant tunneling diode [34]. The resonant tunneling diode has a region in its voltage/current characteristics where the current decreases with increased forward voltage. This property of resonant tunneling diode can be used as a basis of memory, switching mechanism, and logic functionality [35, 36, 37, 38]. Graphene can be used as a field effect transistor where the voltage signal applied to the gate modulates the channel current which is converted into a voltage signal upon passing through a load resistor [39, 40, 41]. The voltage gain of the amplifier depends upon the transconductance of a field effect transistor [FET] and load resistance [39]. A schematic drawing of a FET is shown in figure 8.1. So, FET is an electronic device with at least three terminals [39] and the conductivity between source and drain is modulated by the gate voltage. This gate voltage control such that it acts as switch which conducts high current when it is on and very low current when it is off. Graphene can be used as a detector of special nuclear material [42, 43, 44, 45]. The modeled device architecture is a graphene-based field effect transistor which consists of graphene on a radiation-absorbing, electrically-gated, undoped semiconductor absorber, separated by a thin dielectric buffer layer [42]. The conductivity of FET

abruptly changes by charge carriers produced by radiation which falls upon absorber material.



Figure 8.1: Schematic drawing of a field effect transistor in which graphene is placed between drain and source.

#### 8.3 Summary and Conclusions

The energy per atom of graphene is -1043.496704 eV and the energy per atom of a corresponding nanotube is -1041.976612 eV. This is shown in Table 1. So, the energy per atom in the two cases differs by 0.1456%.

In the case of graphene, in the negative region, the density of states is fluctuating, but beyond that, its value increases sharply from 0 to -1 eV and then decreases around -2 eV. In the positive region of the energy, the density of the states rises up to 2 eV. But in the case of the carbon nanotube with diameter 4.3830 nm, the density of states is rapidly fluctuating, also up to 2 eV. In negative voltage regions, the density of states is also fluctuating but much higher beyond -1 eV. In the case of a nanotube with diameter 3.6129 nm, the density of states increases up to approximately 20/eV in the negative region while it reaches surprisingly a maximum value of 45/eV in the positive region. In the case of the nanotube with diameter 2.4338 nm, the density of states fluctuates in the positive regions of energy with a maximum value of 55 eV<sup>-1</sup> and then decreases to around 5 eV<sup>-1</sup>, whereas in the negative regions of energy, its value is even more fluctuating with a maximum of 60 eV<sup>-1</sup> and then decreases to 11 eV<sup>-1</sup>. So the density of states is also different in the case of graphene and nanotubes.

In the case of graphene, in the region around 0 eV, the transmission coefficient is small, but in the negative region of energy it increases, passes through a maximum and then decreases down to 1eV. In the region of -1eV, the transmission remains low and fluctuating until around -1.4 eV, and then increases and becomes

maximum, and then decreases to around 0.26. But in the case of a nanotube with a diameter 4.3830 nm, the transmission coefficient beyond 0 eV is fluctuating and shows a decreasing trend in the positive region. In the negative region, its curve is still fluctuating, but with an increasing trend. The value of the transmission coefficient is larger at -2 eV than 2 eV. Beyond -1.0 eV, the average values of the transmission coefficient are higher than the average beyond 1.0 eV. In the case of nanotube 3.6129 nm, beyond 1eV, the transmission coefficient is highly fluctuating and then decreases. In the negative voltage region the nature of the transmission coefficient is also fluctuating and reaches to around 3.75 eV and then decreases. In the case of nanotube with diameter with 2.4338 nm, the transmission spectrum is highly fluctuating and has maximum value up to 1.6 and decreases below 0.2 at 2 eV in positive region, whereas the values of transmission coefficients are also fluctuating in negative region and its value reaches to maximum value over 1.6 and decreases to around 0.9 at -2 eV. So the transmission spectrum of graphene and nanotubes is different.

In the case of graphene, the current is fluctuating in the region from 0.5eV to around 1.5 eV and then increases. In the negative region of the bias voltage from – 0.5 eV to -1.5 eV, the current fluctuates little and then increases. But in the case of nanotube with diameter 4.3830 nm, currents are more fluctuating in the positive bias voltages whereas in the negative bias voltage is slightly fluctuating. Around - 1.8 eV, its value is at maximum and then decreases. In the case of nanotube with diameter 3.6129 nm, in the positive region, we find a stronger fluctuation of the current beyond 1V and reaches maximum of 68000 nA, and then decreases. But in

the negative region, there is less pronounced fluctuation in the current and its value reaches around a maximum of 75000 nA, and then slightly decreases. In the case of nanotube with diameter 2.4338 nm, the current fluctuates slowly in the positive region of bias voltage and finally reaches to around 42000 nA, but in negative regions current fluctuates highly and reaches to around 680000 nA. So the trend of current in graphene and nanotubes is different.

- The effective mass of an electron inside graphene is zero at Dirac's points but an electron gains mass when the graphene sheet is folded to form a carbon nanotube.
- The Fermi velocity of an electron in the case of graphene is  $1.1 \times 10^6 m/s$ , but in the case of a nanotube, this value drops by 10% approximately.
- The Klein Paradox is no longer really a paradox when chirality is taken into account.
- The total energy per atom for Pentacene, Dibenz [a,j]anthracene and Picene is -1047.414548 eV, -1047.447088 eV and -1047.446973 eV, respectively as shown in the table 1. Therefore, the total electronic energy per atom of different structural isomers is different.
- Graphene and carbon nanotubes show negative differential resistance which is characterized as a decrease of current with an increase of voltage which is shown while drawing current vs. voltage graphs.

# ✤ Future plan

- A study of the transmission through bilayer and trilayer graphene needs to be done.
- > A study of energy storing capacity of graphene also needs to be done.
- Given the opportunity, I plan to study the following properties of graphene and carbon nanotube:
- Graphene has Young's modulus 1000 GPa but for steel is 200 GPa. Therefore, graphene is more than 5 times stronger than steel.
- Graphene is almost optically transparent and absorbs only 2.3% of light intensity which incidents upon it.
- ★ The graphene sheet has electrical conductivity  $0.96 \times 10^6 \,\Omega^{-1} cm^{-1}$  and electrical conductivity of copper is  $0.60 \times 10^6 \,\Omega^{-1} cm^{-1}$ . Thus, graphene has higher conductivity than copper. Conductivity can be modified over a large rage by doping impurities.
- Thermal conductivity of graphene is around 4840-5300 W/mK and that of silver is 429W/mK. So thermal conductivity of graphene is much higher than silver.
- ✤ The mobility of graphene at room temperature is 200,000 cm<sup>2</sup>V<sup>-1</sup>s<sup>-1</sup> at carrier density of n=  $10^{12}$  cm<sup>-2</sup>. The mobility is very high which can be used for electronic high frequency applications.

- Transistor made of graphene is 10-100 times faster than silicon based transistor.
   Flexible electronics and gas sensors are also other potential applications of it.
- The quantum Hall effect in graphene could possibly contribute to make more accurate resistance in metrology.
- Graphene is capable of absorbing a large amount of hydrogen because of its large surface area, so it can store a large amount of energy.
- Thermal conductivity of a nanotube is very high and ranges from1750 W/mK to 5800 W/mK.
- Electrical conductivity of a nanotube is also very high.
- The Young's modulus of a carbon nanotube can be 1000 GPa which is approximately 5 times higher than steel. Also tensile strength of it can be up to

63 GPa which 50 times higher than steel.

- Under certain condition, we can insert carbon nanotube inside cells and causes death of a cell.
- A carbon nanotube shows semiconducting with very low band gap as well as metallic behavior.
- A carbon nanotube is very useful in the field of nanotechnology. We can make microprocessors as well as micro-transistors. So, a carbon nanotube is supposed to have superior electronic properties than current silicon-based devices.

# 9 Appendices

#### 9.1 Appendix A:

9.1.1 Evaluation of the self-energy



Figure 9.1: 1-D wire to calculate Hamiltonian.

Consider a semi-infinite 1D wire illustrated by a one-band effective mass Hamiltonian of the form shown in the figure. Let us treat the first point of the wire labeled "0" as our channel and the remaining points are labeled n < 0 as the contact.

If the channel were decoupled from the contact, it is described by the equation [17]

$$E\psi = H\psi = (E_c + 2t_0)\psi.$$
 [9.1.1]

Once it is coupled to the contact, this equation is modified to the following equation,

$$E\psi = (E_c + 2t_0)\psi - t_0\phi_{-1}. \qquad [9.1.2]$$

where the contact wave functions  $\phi_n$  satisfies an infinite series of equations n < 0,

$$E\phi_n = -t_0\phi_{n-1} + (E_c + 2t_0)\phi_n - t_0\phi_{n+1}. \qquad [9.1.3]$$

Assuming the solution consists of an incident wave from the contact and a reflected wave back from the channel, we write:

$$\Phi_n = Be^{ikna} + Ce^{-ikna} \,. \tag{9.1.4}$$

Where:

$$E = E_c + 2t_0(1 - \cos ka).$$
 [9.1.5]

Now using equation [9.1.4]

$$\psi = \phi_0 = B + C . \qquad [9.1.6]$$

and,

$$\Phi_{-1} = Be^{-ika} + Ce^{ika} \,. \tag{9.1.7}$$

So that

$$\Phi_{-1} = \Psi e^{ika} + B \left[ e^{-ika} - e^{ika} \right].$$
[9.1.8]

Substituting this expression into equation [9.1.2], we obtain

So, the self-energy can be given by  $\sum = -t_0 e^{ika}$ .

#### 9.1.2 Evaluation of the transmission co-efficient



Figure 9.2: Chain of atoms to evaluate the transmission co-efficient.

#### Scattering theory on a discrete lattice:

Let us consider a discrete lattice with points spaced by spacing "a" with the central cell having an extra potential  $U_0/a$  for the delta function. Now we can start with expression [17] given below

$$E\psi_0 = [E_c + 2t_0 + U_0/a]\psi_0 - t_0\psi_{-1} - t_0\psi_{+1}.$$
 [9.1.10]

We know wave functions are continuous at Z = 0

$$\psi_0 = 1 + r = t. \tag{9.1.11}$$

$$\psi_{+1} = t e^{ika}, \qquad [9.1.12]$$

$$\psi_{-1} = e^{-ka} + re^{ika}, \qquad [9.1.13]$$

So that

$$\psi_{+1} = \psi_0 e^{ika} .$$
  
$$\psi_{-1} = e^{-ka} + re^{ika} = e^{-ka} + (t-1)e^{ika} = -2isinka + \psi_0 e^{ika} .$$
[9.1.14]

Substituting back into equation [9.1.10], we get

$$[E - E_c - 2t_0 - U_0/a]\psi_0 = -t_0 [-2i \sin ka + \psi_0 e^{ika}] - t_0 \psi_0 e^{ika},$$
  
Or 
$$\left[E - E_c - 2t_0 - \frac{U_0}{a} + 2t_0 e^{ika}\right]\psi_0 = 2it_0 \sin ka \qquad [9.1.15]$$

Energy dispersion relation 
$$E = E_c + 2t_0(1 - \cos ka),$$
 [9.1.16]  
 $v = \frac{1}{\hbar} \frac{dE}{dk} = \frac{1}{\hbar} 2t_0 a \sin ka.$ 

Therefore,

$$\hbar v = 2t_0 a \, sinka \,. \tag{9.1.17}$$

Now substituting equation [9.1.16] and equation [9.1.17] into equation [9.1.15], we get

$$\left[E - E_c - 2t_0 - \frac{U_0}{a} + 2t_0(\cos ka + i \sin ka)\right]\psi_0 = 2it_0 \sin ka$$

or 
$$\begin{bmatrix} E - E_c - 2t_0(1 - \cos ka) + 2t_0 i \sin ka - \frac{U_0}{a} \end{bmatrix} \psi_0 = 2it_0 \sin ka$$

So  $\left[2at_0i \ sinka/a - \frac{U_0}{a}\right]\psi_0 = 2it_0a \ sinka/a$ 

$$-\frac{U_0}{a}\psi_0 + \frac{i\hbar v\psi_0}{a} = \frac{i\hbar v}{a}$$

 $\psi_0 = \frac{i\hbar\nu}{i\hbar\nu - U_0} \, .$ 

or

Therefore,

$$t=\frac{i\hbar v}{i\hbar v-U_0} ,$$

Then, the transmission co-efficient  $(E) = |t|^2 = \frac{\hbar^2 v^2}{\hbar^2 v^2 + U_0}$ . [9.1.18]

Green's function method: Hamiltonian of the channel can be given as follows:

$$H = E_c + 2t_0 + U_0/a . [9.1.19]$$

Self-energy of the left contact  $\sum_1 = -t_0 e^{ika}$ .

Self-energy of the right contact  $\sum_2 = -t_0 e^{ika}$ .

Coupling parameter  $\Gamma_{1,2} = i \left[ \sum_{1,2} - \sum_{1,2}^{\dagger} \right] = 2t_0 \ sinka = \hbar v/a.$ 

We know Green's function

$$G = [EI - H - \sum_{1} - \sum_{2}]^{-1} = [E - E_{c} - 2t_{0} + 2t_{0}e^{ika} - U_{0}/a]^{-1}$$
  

$$= [E - E_{c} - 2t_{0} + 2t_{0}(coska + isinka) - U_{0}/a]^{-1}$$
  

$$= [E - E_{c} - 2t_{0}(1 - coska) + 2t_{0}isinka) - U_{0}/a]^{-1}$$
  

$$= [2at_{0}isinka/a - U_{0}/a]^{-1} = [i\hbar v/a - U_{0}/a]^{-1} = \frac{a}{i\hbar v - U_{0}}$$
  

$$T(E) = Tr[\Gamma_{1}G\Gamma_{2}G^{\dagger}] = \frac{\hbar^{2}v^{2}}{\hbar^{2}v^{2} + U_{0}}.$$
[9.1.20]

## 9.2 Appendix B:

9.2.1 Relation between current, voltage, and transmission co-efficient

$$Current I = nev, [9.2.1]$$

where n is the electron density and v is the speed of the electron.

Again,

$$n_j(E) = D_j(E)f(E - \mu_j),$$
 [9.2.2]

Where  $D_j(E)$  the density of state of jth quantum is state and  $f(E - \mu_j)$  is the Fermi function.

Therefore,

$$I(E) = eT(E)[n_s(E)v_s(E) - n_D(E)v_D(E)].$$
[9.2.3]

Where T(E) is the transmission function.

Again,

$$D_j(E) = \frac{1}{2\pi\hbar} \sqrt{\frac{2m^*}{E - E_{1,j}}} .$$
 [9.2.4]

and

$$v_j = \sqrt{\frac{2(E - E_{1,j})}{m^*}} \ . \tag{9.2.5}$$

Plugging these expressions in the equation,

$$I(E) = \frac{eT(E)}{\pi\hbar} [f(E - \mu_S) - f(E - \mu_D)].$$
[9.2.6]

At zero temperature, the Fermi function becomes the Heaviside

step function  $\theta(\mu_j - E)$ .

Therefore,

$$I(E) = \frac{eT(E)}{\pi\hbar} [\Theta(E - \mu_S) - \Theta(E - \mu_D)] dE = \frac{2e^2}{h} TV.$$
 [9.2.75]

#### 9.2.2 Code for graphs

Codes for Transmission probability Vs. Barrier height for graphene

Input1:

gnuplot>

set angles degrees

set xrange[0:300]

set yrange[0.982:1.002]

set xlabel "Barrier height"

set ylabel "Transmission probability"

gnuplot> plot 0.82139/(1-0.1786\*cos(sqrt(80-x)\*0.005765-7.05)\* cos(sqrt(80-

x)\*0.005765-7.05)) w l title "Transmission probability vs. barrier height with phi= 25 degree"

Input 2: codes for Transmission probability vs. Barrier width for graphene

gnuplot>

set angles degrees

set xrange[0:150]

set yrange[0:1.002]

set xlabel "Barrier width"

set ylabel "Transmission coefficient"

gnuplot> plot  $0.75/(1-0.25*\cos(0.56187*x)*\cos(0.56187*x))$  w l title "Transmission Vs barrier width with phi=30 degree and barrier height=450meV", "0.999695/(1-0.000304\*\cos(0.56187\*x)\*\cos(0.56187\*x)) w l title "Transmission Vs barrier width with phi=1 degree and barrier height=450meV"

Input 3: codes for Transmission probability Vs Barrier width for graphene

gnuplot>

set angles degrees

set xrange[0:40]

set yrange[0.9992:1.00001]

set xlabel "Barrier width"

set ylabel "Transmission coefficient"

gnuplot> plot 0.999695/(1-0.000304\*cos(0.56187\*x)\*cos(0.56187\*x)) w l title "

Transmission Vs barrier width with phi=1 degree and barrier height=450meV"

Input 4: codes for Transmission probability Vs Barrier width for graphene

gnuplot>

set angles degrees

set xrange[0:40]

set yrange[0.95:1.01]

set xlabel "Barrier width"

set ylabel "Transmission coefficient"

gnuplot> plot 0.75/(1-0.25\*cos(0.56187\*x)\*cos(0.56187\*x)) w l title "

Transmission Vs barrier width with phi=30 degree and barrier height=450meV"

Input 5: codes for energy vs.  $ak_x$  and  $ak_y$ .

gnuplot>

set xrange[-4:4]

set yrange[-4:4]

set zrange[-3:3]

set pm3d

gnuplot>splot sqrt(1+4\*cos(0.866025\*x)\*cos(1.5\*y)+4\*cos(1.5\*y)\*cos(1.5\*y)), "sqrt(1+4\*cos(0.866025\*x)\*cos(1.5\*y)+4\*cos(1.5\*y)\*cos(1.5\*y))" w l title "Evergy Vs. Wave vector"

Note: Here  $x = ak_x$  and  $y = ak_y$ 

# 10 Chapter

#### 10.1 Presentations

- "Theoretical study of Quadrupole Ion trap and its Application." Seminar in Fall
   2009 in the University of Nevada, Reno.
- "Study of General theory of Relativity and Cosmology." Seminar in Spring 2011 in the University of Nevada, Reno.
- "Detailed Study of Parity violation" in Spring 2011 in the University of Nevada, Reno.
- "Detailed Study of Atomic Clock" in Fall 2011 in the University of Nevada, Reno.
- "Study of Two photon emission" in Spring 2012 in the University of Nevada, Reno.
- "Study of AIDS Virus and its Remedy" in Spring 2012 in the University of Nevada, Reno.
- "Study of Transmission of electric current through structural isomers of C<sub>40</sub>."
   Presentation at the California-Nevada Section of American Physical Society Meeting, Stanford University, CA, November 2011.
- "Study of Entropy of Black Hole by using Hawking's and String Theory."
   Seminar in Fall 2012 in the University of Nevada, Reno.

## References:

[1] Aviram, A. Ratner, M. A., "Molecular rectifiers" Chem. Phys. Lett. 29 (1974) 277.

[2] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov and A. K. Geim, "The electronic properties of graphene, 2009.

[3] H. S. Philip Wong and Deji Akinwande, "Carbon Nanotube and Graphene Device Physics." Cambridge University Press, Cambridge, ISBN: 97805119169532010 page 61, 50, 55, 58, 59, 60.

[4] C. H. Fuentevilla, and J. D. Lejarreta, "Angle dependent Conductance in Graphene" 2010 page 1.

[5] Anton Z. Capri, "Relativistic Quantum mechanics and introduction to Quantum field theory", Published by World Scientific Publishing Co. Pte. Ltd. Farrrer Road, Singapore 912805 ISBN 981-238-137-6 page 8, 17 (2002).

[6] M. I. Katsnelson, K. S. Novoselov and A. K. Geim, "Chiral tunneling and the Klein Paradox in Graphene" page 622(2006).

[7] C. M. Kachhava ,"Solid state Physics", Published by Tata McGraw-Hill, New Delhi 110002 1990, 108

[8] P. R. Wallace, The band theory of graphite. Phys. Rev., 17 (1974)622-34

[9] B. K. Agrawal, Hari Prakash, "Quantum Mechanics" June 2001, Second Edition, Published by Asoke K. Ghosh, Prentice-Hall of India Pvt.Ltd., New Delhi-110020 page 378, 379, 380, 528,

[10] R. Saito, G. Dresselhaus, M. S. Dresselhaus, "Physical Properties of Carbon Nanotubes", Published by Imperial College Press, 57 Shelton Street, Covent Gardon, London WC2H 9HE, ISBN: 1-86094-223-7, 2005, page 37, 38, 61, 64, 39, 40, 47, 60, 61, 75.

[11] Richard D. Mattuck, "A Guide to Feynman Diagrams in the Many-Body Problem", Second Edition, published by McGraw-Hill Book company, New York, page 12, 26, 19, 189, 154.

[12] Jimmie D. Doll, William P. Reinhardt, " $\pi$  Electron Theories Viewed as Parametrizations of the One-Body Green's Function" The Journal of Physical Chemistry,88-11,1509(1979). [13] Satya Prakash, "Advanced Quantum mrchanics" Published by Knrn, India, ISBN: 9788190701167, 2002, page 527, 545, 547.

[14] Paul Roman, "Advanced Quantum Theory", Published by Addson-Wesley Publishing Company, Ing., USA, page 122 (1965)

[15] Lubomir Sodomka, "Strucure and Properties of Solids" page 111(1967), London Iliffe Books Ltd.

[16] Charles Kittel, "Introduction to Solid State Physics" page 120(2006), seventh Edition, John Wiley and Sons, Inc., Singapore, New York, Chichester, Brisbane, Toronto.ISBN 9971-51-180-0

[17] Supriyo Datta, "Quantum transport Atom To Transistor" page 240, 186, 241 (2006), Cambridge University press, New York, ISBN: 0-521-63145-9

[18] Peter W. Higgs, "Broken Symmetries and the Masses of Gauge Bosons", 1964, Vol. 3, Number 16

[19] Giovanni Organtini, "Unveiling The Higgs mechanism to students" European J. of Physics, 2012 page 1399

[20] A.D. Alhaidari, A. Jellal, E.B. Chubabi and H. Bahlouli, "Dynamical mass generation via space compactification in graphene" The university of Saudi Arabia, 2010 page 4.

[21] Rui Yang, Liang Huang, Ying-Cheng Lai, and Celso Grebogi "Abnormal electron paths induced by Klein tunneling in graphene quantum point contacts" 035426- 1(2011)

[22] Andrea F. Young and Philip Kim "Electronic Transport in Graphene Hetrerostuctures" page 102 (2010)

[23] Edward McCann, "Staying or going? Chirality decides" Physics 2, 98 (2009)

[24] Q. Shao, G. Liu, D. Teweldebrhan, and A.A. balandin, "High-temperature quenching of electrical resistance in graphene interconnects," Applied Physics Letter, 2008.

[25] V. Krstic, S. Roth, and M. Burghard, "Localization and nonlinear transport in a single walled carbon nanotube fibres" Phys. Rev. B **62**, R16353 (2000)

[26] W. Liang, M. Bockrath, D. Bozovic, J. Hafner, M. Tinkham, and H. Park, " Electron transport properties of Carbon nanotube-graphene contacts" Nature **411**, 665 (2001). [27] J. Kong, D. Yenilmez, T. Kim, W. Dai, R. Laughlin, L. Liu, C. Jayanthi, and W. Wu, "Electron Transport in Single-Walled Carbon Nanotubes" Phys. Rev. Lett. **87**, 106801 (2001).

[28] X. Blase, Lorin X. Benedict, Eric L. Shirley, and Steven G. Louie, "hybridization Effects and Metallicity in small Radius Carbon Nanotubes" Physical Review Letters, 1994 page 1880

[29] Valentin N. Popov "Carbon nanotubes: properties and application." A Review Journal, 2004

[30] www.substech.com, accessed on December 2012.

[31] nanotech-now.com, ncnr.nist.gov, accessed on December 2012.

[32] Quantumwise "Atomistix Toolkit package", www.quantumwise.com

[33] Ali Nasir Imtani, V.K.Jindal, "Bond Lengths of Single Carbon Nanotubes" Phys. Rev.B, (2006).

[34] Caijuan Xia, Hanchen Liu, Qiuping Wang, "An ab intio study on negative differential resistance in pyrrole trimer molecular device", Advance material Research volumes 152-153(2011) pp931-934.

[35]. Meric, N. Baklitskaya, P. Kim, and K. L. Shepard, "RF performance of top-gated, zerobandgap graphene field-effect transistors," in Int.Electron Devices Meeting Tech. Dig.,

2008, pp. 1-4.

[36] L. Liao, Y.-C. Lin, M. Bao, R. Cheng, J. Bai, Y. Liu, Y. Qu, K. L.Wang, Y. Huang, and X. Duan, "High-speed graphene transistors with self-aligned nanowire gate," Nature, vol. 467, no. 7313, pp. 305–308,2010.

[37] Y.-M. Lin, C. Dimitrakopoulos, K. A. Jenkins, D. B. Farmer, H.-Y. Chiu, A. Grill, and P. Avouris, "100-GHz transistors from wafer-scale epitaxialgraphene," Science, vol. 327, no. 5966, p. 662, 2010.

[38] Y. Wu, Y. ming Lin, A. A. Bol, K. A. Jenkins, F. Xia, D. B. Farmer, Y. Zhu, and P. Avouris, "High-frequency, scaled graphene transistors ondiamond-like carbon," Nature, vol. 472, no. 7341, pp. 74–78, 2011.

[39] Dharmendar Reddy, Leonard F. Register, Gary D Carpenter, Sanjay K. Banerjee, "Graphene field-effect transistors" J. Phys. D. Appl. Phys.44(2011) 313001(20pp).
[40] Novoselov K.S., Geim A.K., Morozov S.V., Jiang D, Zhang Y, Dubonos S.V., Grigorieva I.V., and Firsov A.A., "Electric field effect in atomically thin carbon films", Science 306, no. 5696, pp. 666-669, Oct.2004.

[41] A.K.Geim and K.S.Novoslov, "The rise of graphene," Nat. Mater., vol.6, no.3, pp183-191, Mar.2007.

[42] Michael Foxe, Student Member, IEEE, Gabriel Lopez, Student Member, IEEE, Isaac Childres, Romaneh Jalilian, Amol Patil, Caleb Roecker, John Boguski, Igor Jovanovic, and Yong P. Chen, Member, IEEE, "Graphene Field-Effect Transistors on Undoped Semiconductor Substrates for Radiation Detection" page 581, January 2012.

[43] F. Schedin, A. K. Geim, S. V. Morozov, E. W. Hill, P. Blake, M. I.Katsnelson, and K. S. Novoselov, "Detection of individual gas moleculesadsorbed on graphene," Nat. Mater., vol. 6, no. 9, pp. 652–655, Sep. 2007.

[44] P. Luke and E. Eissler, "Performance of cdznte coplanar-grid gamma-raydetectors," IEEE Trans. Nucl. Sci., vol. 43, no. 3, Part 2, pp. 1481–1486, Jun. 1996.

[45] Z. He, G. Knoll, D. Wehe, and J. Miyamoto, "Position-sensitive single carrier cdznte detectors," Nucl. Instrum. Methods A, vol. 388, no. 1–2,pp. 180–185, Mar. 1997.