ELECTRON OPTICS IN GRAPHENE

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by
Gürcan COŞGEL

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İZMİR

Dedicated to the memory of my beloved father

Mesut COŞGEL

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ABSTRACT

ELECTRON OPTICS IN GRAPHENE

Negative refraction, also known as Veselago lensing, was first predicted by Victor Veselago in 1968 (Veselago (1968)). Its unique effect has a great potential for both scientific and technological applications such as superlenses. Unlike the conventional positive refractive index, focusing effect can be observed by negative refraction. In this thesis, the focusing effect was investigated theoretically through on n-p junction in graphene. The opposite chirality of electrons and holes enable the negative refraction where electrons(holes) have their momentum parallel(anti-parallel) to the group velocity. The case when potential barrier is directed perpendicular to KK' direction, where K and K' are the Dirac points were considered. The Green's functions were calculated analytically and derived the susceptibility using the Green's functions for various positions of the sources and the receiver at various Fermi energies. The spatial Green's functions were calculated analytically and derived the static susceptibility (response function).

ÖZET

GRAFENDE ELEKTRON OPTİĞİ

Negatif kırılma, ayrıca Veselago mercekleme olarak da bilinen, Victor Veselago tarafından 1968'de (Veselago (1968)) öngörülmüştür. Benzersiz etkisi süperlensler gibi hem bilimsel hem de teknolojik uygulamalar için büyük bir potansiyele sahiptir. Geleneksel pozitif kırılma indeksinin aksine, odaklama etkisi negatif kırılma ile gözlemlenebilir. Bu tezde, grafende n-p eklemi üzerinden odaklama etkisi teorik olarak araştırılmıştır. Elektronların ve boşlukların zıt kiralitesi, elektronların(boşlukların) momentumlarının grup hızına paralel(anti-paralel) olduğu durumlarda negatif kırılmaya olanak sağlar. Potansiyel bariyerin Dirac noktaları olan K ve K' doğrultusuna dik olduğu durum değerlendirilmiştir. Green fonksiyonları analitik olarak hesaplanmıştır ve çeşitli Fermi enerjilerinde kaynakların ve alıcıların çeşitli pozisyonları için Green fonksiyonları kullanılarak duyarlılık türetilmiştir. Uzamsal Green fonksiyonları teorik olarak hesaplanmıştır ve statik duyarlılık (tepki fonksiyonu) türetilmiştir.

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CHAPTER 1

INTRODUCTION

Carbon is an extraordinary element in life. It appears in various forms such as protein. This is the reason of its ability in terms of flexible bonding due to its four valance electrons. Well-known allotropes of the carbon atom are graphite, diamond and graphene. Graphene is of great importance to understand the electronic properties of the allotropes of the carbon atom and synthesized by Novoselov (Novoselov et al. (2004)). It is the two-dimensional allotrope of the carbon atom and single layer material that has hexagonal lattice structure with sp^2 hybridization (also known as honeycomb lattice because of the shape). Because the behaviour of the mobile electrons in graphene, they treated as massless relativistic particles to comprehend the remarkable electronic properties (Novoselov et al. (2012); Geim and Novoselov (2007); Choi et al. (2010); Castro Neto et al. (2009)).

Veselago Lens is validation of negative refractive index of a material and first found by Soviet/Russian physicist Victor Veselago (Veselago (1968)). He found the occurrence of the negative index of refraction if the permittivity and the permeability are negative. After, comfirmation was done by David Smith et al. (R. A. Shelby et al. (2001)) and Pendry (Pendry (2004)) experimentally. Researches show that this effect can be examined by constructing n-p junction in graphene but also some other variations (Cheianov et al. (2007); Chen et al. (2016); Reijnders and Katsnelson (2017a); Cserti et al. (2007); Libisch et al. (2017); Farhi and Bergman (2014); Hills et al. (2017); Lee et al. (2015)). In this work, Veselago Lens effect is investigated. The motivation is to observe this effect in graphene theoretically and find the susceptibility.

1.1. Graphene

Lattice structure of the graphene is hexagonal as shown in fig. 1.1 and contains two sublattices, called A and B, in the unit cell.

Due to the symmetry, sublattices can be chosen arbitrarily. Unit vectors of the lattice are $\vec{a}_1$ and $\vec{a}_2$ (Kittel (2004); Katsnelson (2012));

$$\vec{a}_1 = \frac{a}{2}(3, \sqrt{3}) \qquad \vec{a}_2 = \frac{a}{2}(3, -\sqrt{3}) \tag{1.1}$$

where the distance between two atoms, a, is 1.42 Å. Nearest neighbor vectors are δ vectors in fig 1.1 shows the positions of the nearest neighbor sublattice atoms of B.

$$\vec{\delta}_1 = -\frac{a}{2}(1, 0) \qquad \vec{\delta}_2 = \frac{a}{2}(1, -\sqrt{3}) \qquad \vec{\delta}_1 = \frac{a}{2}(1, \sqrt{3}) \tag{1.2}$$

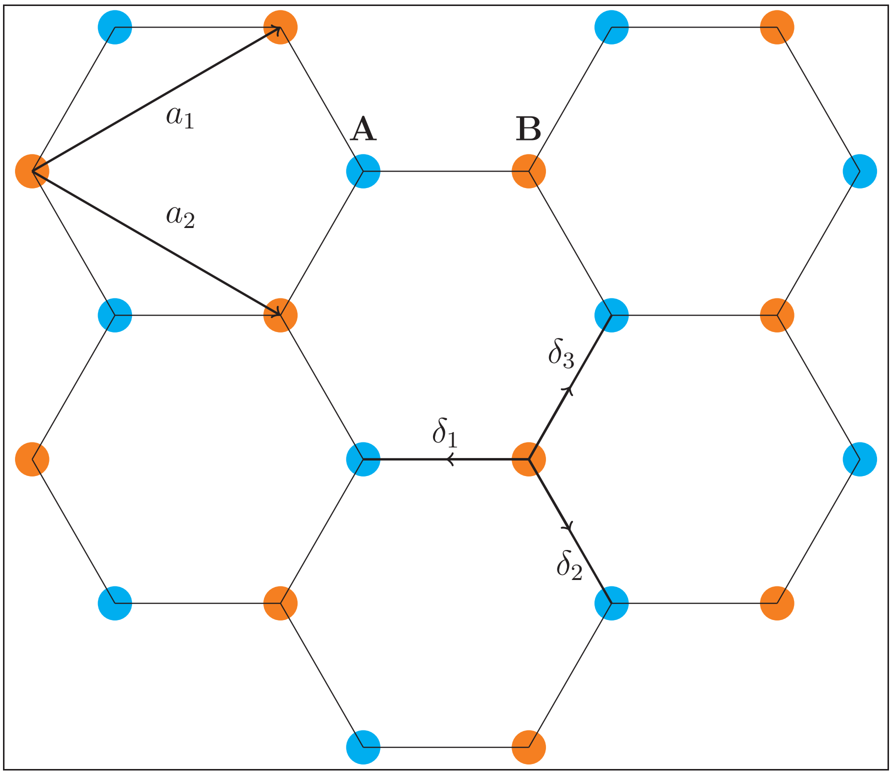


Figure 1.1. Honeycomb shape structure of the graphene, sublattices A and B are cyan and orange colored respectively. Nearest neighbor vectors are indicated as δ_1, δ_2, and δ_3

Reciprocal lattice vectors are shown in fig 1.2 which are;

$$\vec{b}_1 = \frac{2\pi}{3a}(1, \sqrt{3}) \qquad \vec{b}_2 = \frac{2\pi}{3a}(1, -\sqrt{3}) \tag{1.3}$$

Γ, M, K and K' are the special points in terms of high symmetry in the Brillouin zone as shown in fig. 1.2. K and K' points have special names called Dirac points and the vectors show their positions are;

$$\vec{K} = \left(\frac{2\pi}{3a}, \frac{2\pi}{3\sqrt{3}a}\right) \qquad \vec{K'} = \left(\frac{2\pi}{3a}, -\frac{2\pi}{3\sqrt{3}a}\right) \tag{1.4}$$

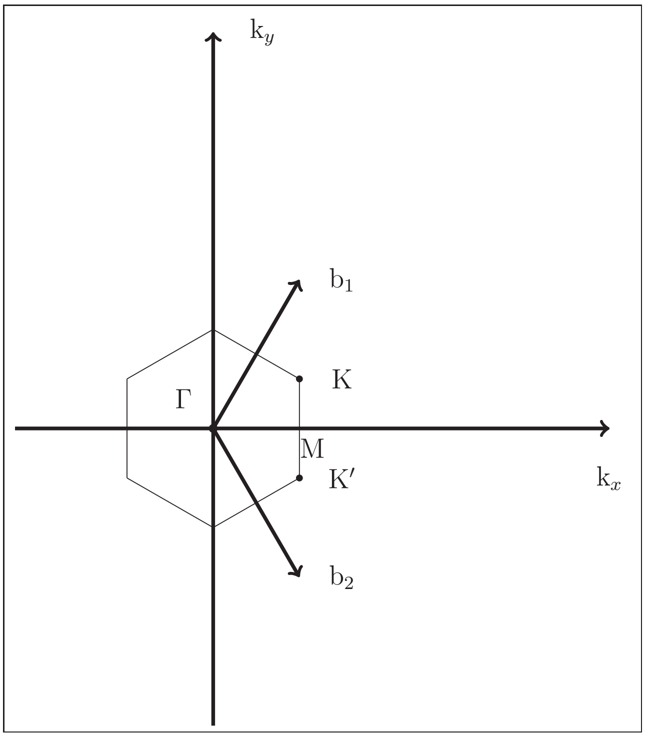


Figure 1.2. In momentum space, Brillouin zone has special points K and K' points called Dirac points. $\vec{b}_1$ and $\vec{b}_2$ are reciprocal lattice vectors in Brillouin zone.

These points are characteristic of electronic structure of graphene and obtained by Wallace (Wallace (1947); Bena (2009); Güçlü et al. (2014); Saito et al. (1998); Reich et al. (2002)) with simple tight-binding model then McClure (McClure (1957)) and Slonczewski & Weiss (Slonczewski and Weiss (1958)) developed this model. Tight-binding model is used to express the nature of unpaired electrons. To do this, following vectors can be used to describe all real points in the lattice.

$$\vec{R}_A = n\vec{a}_1 + m\vec{a}_2 + \vec{b} \tag{1.5}$$

$$\vec{R}_B = n\vec{a}_1 + m\vec{a}_2 \tag{1.6}$$

$\vec{a}_1$ and $\vec{a}_2$ are the primitive lattice vectors, n and m are integers. The vector between A and B sublattices is b. The wavefunctions for A and B sublattices can be written as

$$\Psi_k^A(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{R}_A} e^{i\vec{k}\cdot\vec{R}_A} \psi(\vec{r} - \vec{R}_A) \tag{1.7}$$

$$\Psi_k^B(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{R}_B} e^{i\vec{k}\cdot\vec{R}_B} \psi(\vec{r} - \vec{R}_B) \tag{1.8}$$

The total wavefunction can be written the linear combination of Ψ^A and Ψ^B

$$\Psi_k(\vec{r}) = \alpha\Psi_k^A + \beta\Psi_k^B \tag{1.9}$$

α and β can be determined by diagonalizing the Hamiltonian, where the Hamiltonian is.

$$\hat{H} = \frac{p^2}{2m} + V(r) \tag{1.10}$$

Here $V(r)$ is the atomic potential. Therefore, the Hamiltonian is;

$$\hat{H}(\vec{k}) = \begin{pmatrix} \left\langle \Psi_k^A|\hat{H}|\Psi_k^A \right\rangle & \left\langle \Psi_k^A|\hat{H}|\Psi_k^B \right\rangle \\ \left\langle \Psi_k^B|\hat{H}|\Psi_k^A \right\rangle & \left\langle \Psi_k^B|\hat{H}|\Psi_k^B \right\rangle \end{pmatrix} \tag{1.11}$$

For nearest neighbor approximation, we can assume that $\epsilon_A(\vec{k}) = 0$ and neglect the onside energies which are $\left\langle \Psi_k^A|\hat{H}|\Psi_k^A \right\rangle$ and $\left\langle \Psi_k^B|\hat{H}|\Psi_k^B \right\rangle$.

$$\left\langle \Psi_k^A|\hat{H}|\Psi_k^B \right\rangle = \frac{1}{N} \sum_{\vec{R}_A,\vec{R}_B} e^{i\vec{k}\cdot(\vec{R}_B-\vec{R}_A)} \int d^2r \quad \psi^*(\vec{r}-\vec{R}_A)\hat{H}\psi(\vec{r}-\vec{R}_B) \tag{1.12}$$

Because A and B are nearest neighbor atoms, the integral above is constant. The hopping parameter, which is approximately -2.8 eV can be defined as

$$t \equiv \int d^2r \quad \psi^*(\vec{r}-\vec{R}_A)\hat{H}\psi(\vec{r}-\vec{R}_B) \tag{1.13}$$

Eq. 1.12 and its Hermitian conjugate can be written in terms of hopping parameter as

$$\left\langle \Psi_k^A|\hat{H}|\Psi_k^B \right\rangle = t \sum_{\vec{R}_A,\vec{R}_B} e^{i\vec{k}\cdot(\vec{R}_B-\vec{R}_A)} = t\left(e^{-i\vec{k}\cdot\vec{b}} + e^{-i\vec{k}\cdot(\vec{b}-\vec{a}_1)} + e^{-i\vec{k}\cdot(\vec{b}-\vec{a}_2)}\right) \tag{1.14}$$

$$\left\langle \Psi_k^B|\hat{H}|\Psi_k^A \right\rangle = t \sum_{\vec{R}_A,\vec{R}_B} e^{i\vec{k}\cdot(\vec{R}_A-\vec{R}_B)} = t\left(e^{i\vec{k}\cdot\vec{b}} + e^{i\vec{k}\cdot(\vec{b}-\vec{a}_1)} + e^{i\vec{k}\cdot(\vec{b}-\vec{a}_2)}\right) \tag{1.15}$$

where $f(\vec{k})$ is defined as

$$f(\vec{k}) \equiv e^{-i\vec{k}\cdot\vec{b}} + e^{-i\vec{k}\cdot(\vec{b}-\vec{a}_1)} + e^{-i\vec{k}\cdot(\vec{b}-\vec{a}_2)} \tag{1.16}$$

Energy eigenvalues and eigenfunctions can be found by solving equation below

$$E(\vec{k}) = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = t \begin{pmatrix} 0 & f(\vec{k}) \\ f^*(\vec{k}) & 0 \end{pmatrix} \tag{1.17}$$

$$E_{\pm}(\vec{k}) = \pm|tf(\vec{k})| \tag{1.18}$$

$$\Psi_k^+(\vec{r}) = \frac{1}{\sqrt{2N}} \left(\sum_{RA} e^{i\vec{k}\cdot(\vec{R}_A)} \psi(\vec{r} - \vec{R}_A) - \sum_{\vec{R}_B} e^{i\vec{k}\cdot(\vec{R}_B)} \frac{f^*(\vec{k})}{|f(\vec{k})|} \psi(\vec{r} - \vec{R}_B) \right) \tag{1.19}$$

$$\Psi_k^-(\vec{r}) = \frac{1}{\sqrt{2N}} \left(\sum_{RA} e^{i\vec{k}\cdot(\vec{R}_A)} \psi(\vec{r} - \vec{R}_A) + \sum_{\vec{R}_B} e^{i\vec{k}\cdot(\vec{R}_B)} \frac{f^*(\vec{k})}{|f(\vec{k})|} \psi(\vec{r} - \vec{R}_B) \right) \tag{1.20}$$

Plus sign refers to the solution for the conduction band and the negative sign refers to the solution for the valence band. If we expand the energy dispersion $E(\vec{k})$ around $\vec{K} = (2\pi/3a, 2\pi/3\sqrt{3}a)$ and $\vec{K}' = (2\pi/3a, -2\pi/3\sqrt{3}a)$ with q which is k-space vectors that measured from K and K' respectively, we get

$$f(\vec{K} + \vec{q}) \approx -\frac{3}{2}a(q_x - iq_y) \tag{1.21}$$

$$f(\vec{K}' + \vec{q}) \approx -\frac{3}{2}a(q_x + iq_y) \tag{1.22}$$

$$E_K(\vec{q}) = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = -\frac{3}{2}ta \begin{pmatrix} 0 & q_x - iq_y \\ q_x + iq_y & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \tag{1.23}$$

$$E_{K'}(\vec{q}) = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = -\frac{3}{2}ta \begin{pmatrix} 0 & q_x + iq_y \\ q_x - iq_y & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \tag{1.24}$$

After diagonalization, eigenenergies and wave functions are found as (with changing indices $+ \to c$ and $- \to v$)

$$E^c(\vec{q}) = +\frac{3}{2}a|t||q| \tag{1.25}$$

$$E^v(\vec{q}) = -\frac{3}{2}a|t||q| \tag{1.26}$$

$$\Psi_K^c = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{i\theta} \end{pmatrix} \tag{1.27}$$

$$\Psi_K^v = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -e^{i\theta} \end{pmatrix} \tag{1.28}$$

$\theta = arctan(q_y/q_x))$ is the angle between q_x and q_y. If we introduce the Fermi velocity, $v_F = 3|t|a/2\hbar$, Hamiltonian for the effective mass can be written as

$$\hat{H}_K = -iv_F\vec{\sigma} \cdot \boldsymbol{\nabla} \tag{1.29}$$

$$\hat{H}_{K'} = -iv_F\vec{\sigma}^* \cdot \boldsymbol{\nabla} \tag{1.30}$$

1.2. Veselago lens effect

The Veselago lensing can be investigated by constructing n-p junction as seen in fig.2.1b and fig.2.1a. This is a boundary between n-type and p-type materials where n refers to ”negative” or electrons and p refers to ”positive” or holes respectively. It can be created with electrostatic gates providing control of local doping (Cheianov et al. (2007)). In fig. 1.3, ideal lensing effect is shown. When source is at $x = -1$, expected focusing is at $x = 1$. When $x < 0$, there are electron-like fermions so have positive group velocity and positive momenta. When $x > 0$, there are hole-like fermions so have positive group velocity but negative momenta. On the n-side of the junction, flow of the electrons is divergent. On the other side of the junction, flow is convergent. That is why focusing effect can be seen, especially under the symmetric condition that is the source is at $x = -1$ and receiver is at $x = 1$.

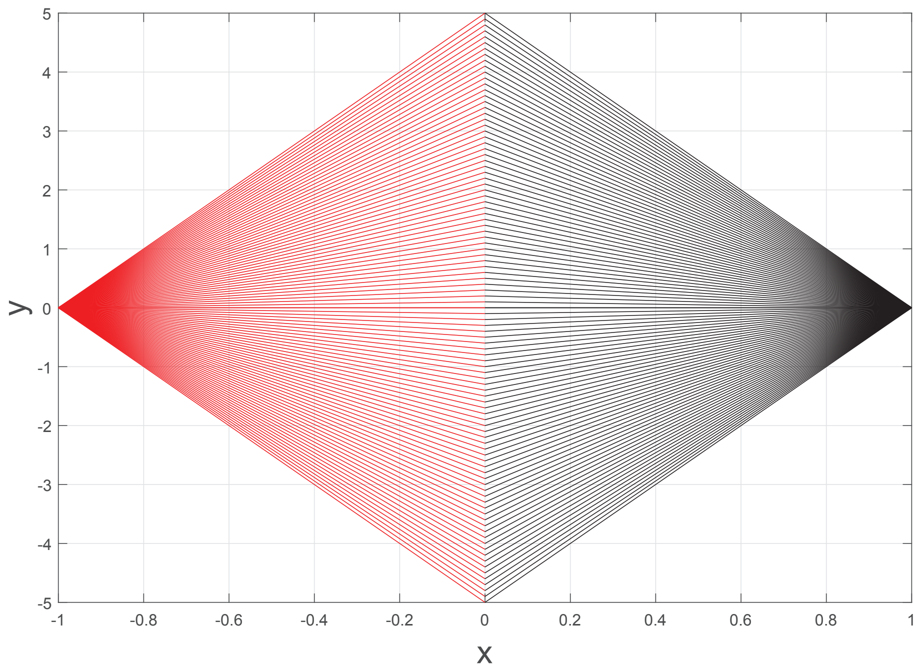


Figure 1.3. Veselago lens effect when source is at $x = -1$.

1.3. Susceptibility

Susceptibility is related to the response of a system to external perturbations (Wolfgang and Anupuru (2016)). In this study, the effect of the perturbation is investigated by constructing n-p junction with different potential values. Specifically, a perturbation which act as a source on n-type side and the response to the perturbation on the p-type side is observed. The effect of perturbation $V(\vec{r}')$ on electron density can be calculated as follows from the Dyson equation (Sherafati and Satpathy (2011); Jishi (2004)) $G = G^0 + G^0 V G$

$$n(\vec{r}) = n_0(\vec{r}) + \int d^3r' \quad \chi(\vec{r},\vec{r}')V(\vec{r}') \tag{1.31}$$

Charge density is defined as

$$n_\mu(\vec{r}) = -\frac{2}{\pi}\int_{-\infty}^{E_F} dE \quad ImG_{\mu\mu}(\vec{r},\vec{r},E) \tag{1.32}$$

exchange interaction between electrons which are located at (μ, r) and (ν, r') can be calculated by finding the charge difference $\delta n_\mu(\vec{r})$ as follows

$$\delta n_\mu(\vec{r}) = -\frac{2}{\pi}Im\int_{-\infty}^{E_F} dE \int d^3r' \quad G^0_{\mu\nu}(\vec{r},\vec{r}',E)V(\vec{r}')G^0_{\nu\mu}(\vec{r}',\vec{r},E) \tag{1.33}$$

here sublattice indices denoted by μ and ν, r and r' are the positions of the magnetic centers. Susceptibility can be obtained by $\delta n_\mu(\vec{r})/\delta V_\nu(\vec{r}')$

$$\chi_{\mu\nu}(\vec{r},\vec{r}') = \frac{\delta n_\mu(\vec{r})}{\delta V_\nu(\vec{r}')} = -\frac{2}{\pi}Im\int_{-\infty}^{E_F} dE \quad G^0_{\mu\nu}(\vec{r},\vec{r}',E)G^0_{\nu\mu}(\vec{r}',\vec{r},E) \tag{1.34}$$

CHAPTER 2

SUSCEPTIBILITY CALCULATIONS

Standard susceptibility for a spin-independent perturbation is written in terms of unperturbed retarded Green's functions (Sherafati and Satpathy (2011))

$$\chi(\vec{r},\vec{r}\,') = -\frac{2}{\pi}\int_{-\infty}^{E_F} dE \quad Im[G^0(\vec{r},\vec{r}\,',E)G^0(\vec{r}\,',\vec{r},E)] \tag{2.1}$$

G^0 is the spin-independent Green's function. For the graphene, we can write the susceptibility as

$$\chi_{\mu\nu}(\vec{r},\vec{r}\,') = -\frac{2}{\pi}\int_{-\infty}^{E_F} dE \quad Im[G^0_{\mu\nu}(\vec{r},\vec{r}\,',E)G^0_{\nu\mu}(\vec{r}\,',\vec{r},E)] \tag{2.2}$$

μ and ν refer to A or B sublattice indices, r and $r\,'$ are the lattice positions on the sublattice μ and ν, respectively. Real-space Green's functions can be determined by integrating the momentum-space Green's functions

$$G^0_{\mu\nu}(\vec{r},\vec{r}\,',E) = \frac{1}{\Omega_{BZ}}\int d^2k \quad e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')}G^0_{\mu\nu}(k,E) \tag{2.3}$$

where $G^0 = (E + i\eta - \mathcal{H}_0)^{-1}$, $\vec{r}$ and $\vec{r}\,'$ are the positions of the atoms. Integral in eq. 2.3 for small energies can be written as

$$G^0_{\mu\nu}(\vec{r},\vec{r}\,',E) = \frac{1}{\Omega_{BZ}}\int d^2k \quad e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')}[G^0_{\mu\nu}(\vec{K},E)e^{i\vec{K}\cdot(\vec{r}-\vec{r}\,')} + G^0_{\mu\nu}(\vec{K}\,',E)e^{i\vec{K}\,'\cdot(\vec{r}-\vec{r}\,')}] \tag{2.4}$$

here K and $K\,'$ are the Dirac points.

In this problem, we have non-homogeneous differential equation as;

$$(E - \hat{H}_K)G(\vec{r} - \vec{r}') = \delta(\vec{r} - \vec{r}') \tag{2.5}$$

Solutions of this non-homogeneous differential equation is Green's functions as a 2×2 matrix

$$G(\vec{r} - \vec{r}') = \begin{pmatrix} G^{AA} & G^{AB} \\ G^{BA} & G^{BB} \end{pmatrix} \tag{2.6}$$

In this problem, low-energy Hamiltonian can be written around K and K' points as

$$\hat{H}_K = v_F \vec{\sigma} \cdot \vec{p} = \begin{pmatrix} 0 & v_F \hat{p}_- \\ v_F \hat{p}_+ & 0 \end{pmatrix} \tag{2.7}$$

$$\hat{H}_{K'} = v_F \vec{\sigma}^* \cdot \vec{p} = \begin{pmatrix} 0 & v_F \hat{p}_+ \\ v_F \hat{p}_- & 0 \end{pmatrix} \tag{2.8}$$

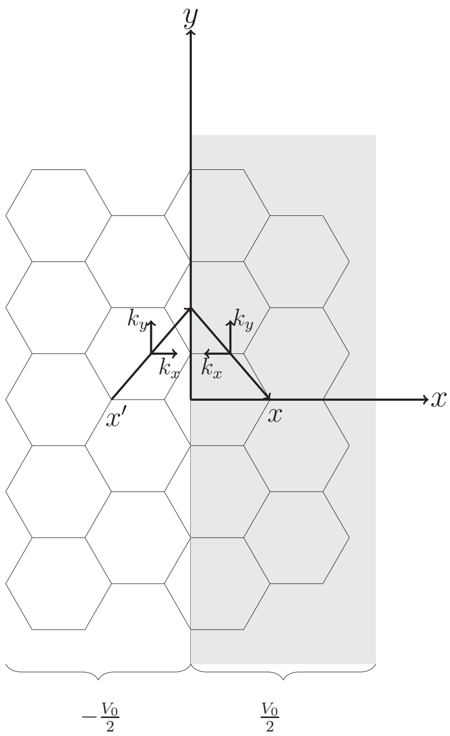
Matrices are the Dirac matrices in two dimensions. Since the effective mass of electrons in graphene is zero, this leads to the Klein tunneling. This means that electrons act like massless Dirac fermions. Under the effect of potential which is simply step potential, Hamiltonian can be written as

$$\hat{H}_K = V + v_F \vec{\sigma} \cdot \vec{p} = \begin{pmatrix} V & v_F \hat{p}_- \\ v_F \hat{p}_+ & V \end{pmatrix} \tag{2.9}$$

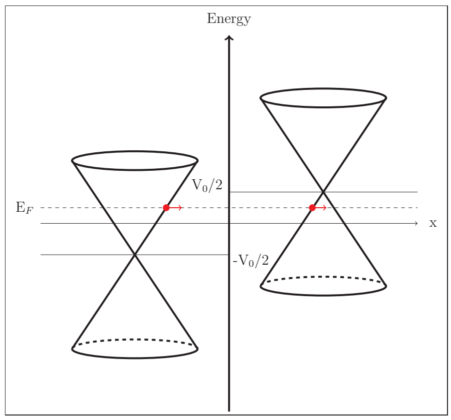
$$\hat{H}_{K'} = V + v_F \vec{\sigma}^* \cdot \vec{p} = \begin{pmatrix} V & v_F \hat{p}_+ \\ v_F \hat{p}_- & V \end{pmatrix} \tag{2.10}$$

The problem can be divided into two based on the step potential barrier as seen in fig 2.1a.

$$V(x) = \begin{cases} -\dfrac{V_0}{2}, & x < 0 \\ \\ \dfrac{V_0}{2}, & x > 0 \end{cases} \tag{2.11}$$



(a)



(b)

Figure 2.1. (a) The incident conduction electron is transmitted as a valance electron whose momentum is in opposite direction to its group velocity. (b) Schematic representation of step potential. Dirac cone for electrons is left side of the barrier (called n-doped or electron-like region), that for holes is right side of the barrier (called p-doped or hole-like region).

The non-homogeneous equation for G^{AA} can be written as

$$(E-V)G^{AA} - |v_F|^2 \hat{p}_- \frac{1}{(E-V)} \hat{p}_+ G^{AA} = \delta(\vec{r}-\vec{r}') \tag{2.12}$$

where

$$\vec{\sigma} = \hat{\sigma}_x \hat{\imath} + \hat{\sigma}_y \hat{\jmath} \tag{2.13}$$

$$\vec{p} = \hat{p}_x \hat{\imath} + \hat{p}_y \hat{\jmath} \tag{2.14}$$

$$\hat{H}_K = \begin{pmatrix} V & v_F \hat{p}_- \\ v_F \hat{p}_+ & V \end{pmatrix} \tag{2.15}$$

where

$$\hat{p}_- = \hat{p}_x - i\hat{p}_y \tag{2.16}$$

$$\hat{p}_+ = \hat{p}_x + i\hat{p}_y \tag{2.17}$$

$$(E - \hat{H}_K) = \begin{pmatrix} E-V & -v_F \hat{p}_- \\ -v_F \hat{p}_+ & E-V \end{pmatrix} \tag{2.18}$$

$$\begin{pmatrix} E-V & -v_F \hat{p}_- \\ -v_F \hat{p}_+ & E-V \end{pmatrix} \begin{pmatrix} G^{AA} & G^{AB} \\ G^{BA} & G^{BB} \end{pmatrix} = \begin{pmatrix} \delta(\vec{r}-\vec{r}') & 0 \\ 0 & \delta(\vec{r}-\vec{r}') \end{pmatrix} \tag{2.19}$$

We have four equations for Green's Functions below

$$(E-V)G^{AA} - v_F \hat{p}_- G^{BA} = \delta(\vec{r}-\vec{r}') \tag{2.20}$$

$$(E-V)G^{AB} - v_F \hat{p}_- G^{BB} = 0 \tag{2.21}$$

$$-v_F \hat{p}_+ G^{AA} + (E-V)G^{BA} = 0 \tag{2.22}$$

$$-v_F \hat{p}_+ G^{AB} + (E-V)G^{BB} = \delta(\vec{r}-\vec{r}') \tag{2.23}$$

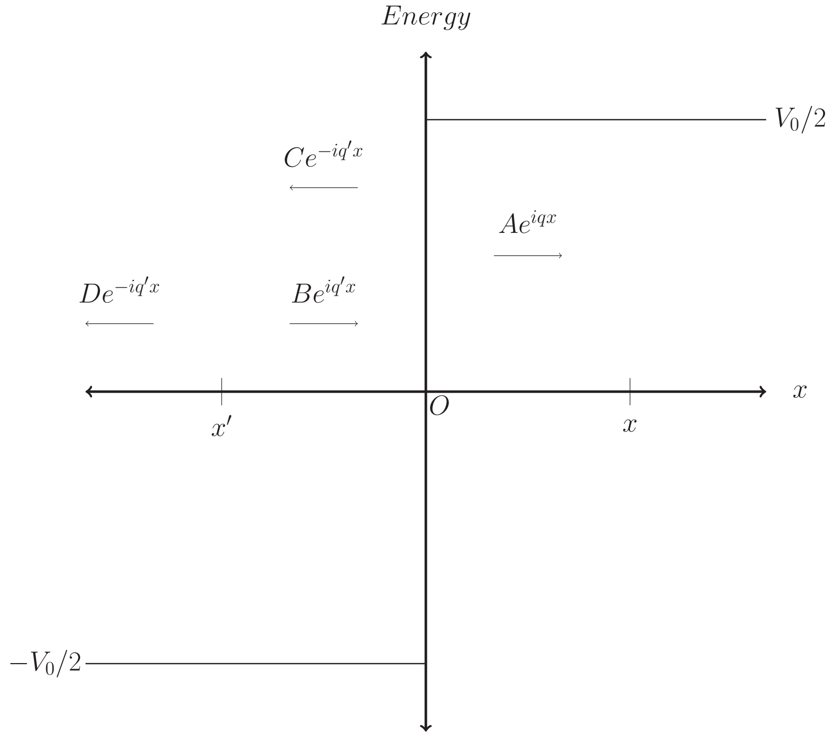


Figure 2.2. Figure shows schematic representation of step barrier potential. Transmitted and reflected waves have wave vectors q on the p-type side and q' n-type side respectively.

If we solve for G^{AA} we get

$$(E-V)G^{AA} - |v_F|^2\hat{p}_-\frac{1}{(E-V)}\hat{p}_+G^{AA} = \delta(\vec{r}-\vec{r}') \tag{2.24}$$

For the conditions below in one-dimension, Green's functions can be found in three regions also shown in fig. (2.2) as

i) $x > 0, \quad x' < 0, \quad -\frac{V}{2} < E < \frac{V}{2}, \quad V > 0$

$$(E-V)G_K^{AA} - (-i\frac{\partial}{\partial x} - ik)\frac{\hbar^2 v_F^2}{(E-V)}(-i\frac{\partial}{\partial x} + ik)G_K^{AA} = \delta(x-x') \tag{2.25}$$

$$x > 0 \quad G_{K_1}^{AA} = Ae^{iqx} \tag{2.26}$$

$$x' < x < 0 \quad G_{K_2}^{AA} = Be^{iq'x} + Ce^{-iq'x} \tag{2.27}$$

$$x < x' < 0 \quad G_{K_3}^{AA} = De^{-iq'x} \tag{2.28}$$

Boundary conditions are;

$$(i) \quad x = x' \tag{2.29}$$

$$(ii) \quad \frac{\partial G_K^{AA}}{\partial x}\bigg|_{x=x'-\epsilon}^{x=x'+\epsilon} = 1 \tag{2.30}$$

$$(iii) \quad x = 0 \tag{2.31}$$

$$(iv) \quad \frac{\partial G_K^{AA}}{\partial x}\bigg|_{x=0-\epsilon}^{x=0+\epsilon} = 0 \tag{2.32}$$

After some algebra, G_K^{AA} can be found as;

$$G_K^{AA} = \frac{(E^2 - \frac{V^2}{4})}{\hbar^2 v_F^2(-kV + iE(q+q') + i\frac{V}{2}(q-q'))} \quad e^{iqx-iq'x'} \tag{2.33}$$

$$G_{K'}^{AA} = \frac{(E^2 - \frac{V^2}{4})}{\hbar^2 v_F^2(kV + iE(q+q') + i\frac{V}{2}(q-q'))} \quad e^{iqx-iq'x'} \tag{2.34}$$

Where;

$$q = -\sqrt{\frac{\left(E - \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2} \tag{2.35}$$

$$q' = \sqrt{\frac{\left(E + \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2} \tag{2.36}$$

To find Green's function for K and K' points, stationary phase approximation method (Reijnders et al. (2018)) is used around $k = 0$ point.

$$\int dk \quad e^{iS} f(k) = e^{iS_0} \quad \sqrt{\frac{i\pi}{S_2}} \quad f(k(x,y)) \tag{2.37}$$

$$\Rightarrow G_K^{AA}(\mathbf{x} > 0, \mathbf{x}' < 0) = \int dk \quad e^{iS} G_K^{AA} \tag{2.38}$$

where S_0 and S_2 are in eq (A.98) and (A.99) respectively

$$G_K^{AA}(\mathbf{x} > 0, \mathbf{x}' < 0) = \frac{\left(E^2 - \frac{V^2}{4}\right) e^{i\left(-\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x - \sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x'\right)} \sqrt{\frac{2i\pi}{\frac{x}{\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} + \frac{x'}{\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}}}}}{\hbar^2 v_F^2 \left((-iE - i\frac{V}{2})\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} + (iE - i\frac{V}{2})\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} \right)} \tag{2.39}$$

$$G_{K'}^{AA}(\mathbf{x} > 0, \mathbf{x}' < 0) = \frac{\left(E^2 - \frac{V^2}{4}\right) e^{i\left(-\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x - \sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x'\right)} \sqrt{\frac{2i\pi}{\frac{x}{\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} + \frac{x'}{\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}}}}}{\hbar^2 v_F^2 \left((-iE - i\frac{V}{2})\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} + (iE - i\frac{V}{2})\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} \right)} \tag{2.40}$$

After interchanging the positions of the source and receiver, we can calculate the Green's functions for K and K' points as

$$G_K'^{AA} = \frac{(E^2 - \frac{V^2}{4})}{\hbar^2 v_F^2(-kV + iE(q+q') + i\frac{V}{2}(q-q'))} \quad e^{iqx'-iq'x} \tag{2.41}$$

$$G_{K'}'^{AA} = \frac{(E^2 - \frac{V^2}{4})}{\hbar^2 v_F^2(kV + iE(q+q') + i\frac{V}{2}(q-q'))} \quad e^{iqx'-iq'x} \tag{2.42}$$

Where;

$$q = -\sqrt{\frac{\left(E - \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2} \tag{2.43}$$

$$q' = \sqrt{\frac{\left(E + \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2} \tag{2.44}$$

$$G_K^{AA}(\mathbf{x'} < 0, \mathbf{x} > 0) = \frac{\left(E^2 - \frac{V^2}{4}\right) e^{i\left(-\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x - \sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x'\right)} \sqrt{\frac{2i\pi}{\frac{x}{\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} + \frac{x'}{\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}}}}}{\hbar^2 v_F^2 \left((-iE - i\frac{V}{2})\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} + (iE - i\frac{V}{2})\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}\right)} \tag{2.45}$$

$$G_{K'}^{AA}(\mathbf{x'} < 0, \mathbf{x} > 0) = \frac{\left(E^2 - \frac{V^2}{4}\right) e^{i\left(-\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x - \sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x'\right)} \sqrt{\frac{2i\pi}{\frac{x}{\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} + \frac{x'}{\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}}}}}{\hbar^2 v_F^2 \left((-iE - i\frac{V}{2})\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} + (iE - i\frac{V}{2})\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}\right)} \tag{2.46}$$

Below the potential value $E < -V/2$, particles act as hole-like fermions. Green's functions for K and K' points are;

$$G_K^{AA} = \frac{(E^2 - \frac{V^2}{4})}{\hbar^2 v_F^2(-kV + iE(q+q') + i\frac{V}{2}(q-q'))} \quad e^{iqx - iq'x'} \tag{2.47}$$

$$G_{K'}^{AA} = \frac{(E^2 - \frac{V^2}{4})}{\hbar^2 v_F^2(kV + iE(q+q') + i\frac{V}{2}(q-q'))} \quad e^{iqx - iq'x'} \tag{2.48}$$

Where;

$$q = -\sqrt{\frac{\left(E - \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2} \tag{2.49}$$

$$q' = -\sqrt{\frac{\left(E + \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2} \tag{2.50}$$

$$G_K^{AA}(\mathbf{x} > 0, \mathbf{x'} < 0) = \frac{\left(E^2 - \frac{V^2}{4}\right) e^{i\left(-\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x + \sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x'\right)} \sqrt{\frac{2i\pi}{\frac{x}{\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} - \frac{x'}{\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}}}}}{\hbar^2 v_F^2 \left((-iE - i\frac{V}{2})\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} + (-iE + i\frac{V}{2})\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}\right)} \tag{2.51}$$

$$G^{AA}_{K'}(\mathbf{x} > 0, \mathbf{x'} < 0) = \frac{\left(E^2 - \frac{V^2}{4}\right) e^{i\left(-\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x + \sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x'\right)} \sqrt{\frac{2i\pi}{\frac{x}{\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} - \frac{x'}{\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}}}}}{\hbar^2 v_F^2 \left((-iE - i\frac{V}{2})\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} + (-iE + i\frac{V}{2})\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} \right)} \tag{2.52}$$

After interchanging the positions of the source and receiver, we can calculate the Green's functions for K and K' points as

$$G'^{AA}_{K} = \frac{(E^2 - \frac{V^2}{4})}{\hbar^2 v_F^2(-kV + iE(q+q') + i\frac{V}{2}(q-q'))} \quad e^{iqx' - iq'x} \tag{2.53}$$

$$G'^{AA}_{K'} = \frac{(E^2 - \frac{V^2}{4})}{\hbar^2 v_F^2(kV + iE(q+q') + i\frac{V}{2}(q-q'))} \quad e^{iqx' - iq'x} \tag{2.54}$$

Where;

$$q = -\sqrt{\frac{\left(E - \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2} \tag{2.55}$$

$$q' = -\sqrt{\frac{\left(E + \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2} \tag{2.56}$$

$$G^{AA}_{K}(\mathbf{x'} < 0, \mathbf{x} > 0) = \frac{\left(E^2 - \frac{V^2}{4}\right) e^{i\left(\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x - \sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x'\right)} \sqrt{\frac{2i\pi}{-\frac{x}{\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} + \frac{x'}{\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}}}}}{\hbar^2 v_F^2 \left((-iE - i\frac{V}{2})\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} + (-iE + i\frac{V}{2})\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} \right)} \tag{2.57}$$

$$G_{K'}^{AA}(\mathbf{x}' < 0, \mathbf{x} > 0) = \frac{\left(E^2 - \frac{V^2}{4}\right) e^{i\left(\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x - \sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x'\right)} \sqrt{\frac{2i\pi}{-\frac{x}{\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} + \frac{x'}{\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}}}}}{\hbar^2 v_F^2 \left((-iE - i\frac{V}{2})\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} + (-iE + i\frac{V}{2})\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}\right)} \tag{2.58}$$

Other component of the Green's function which is BA(AB) is

$$G_K^{BA} = \frac{\hbar v_F q}{\left(E - \frac{V}{2}\right)} G_K^{AA} \tag{2.59}$$

After calculating all the Green's functions, which all are same, we can find the susceptibility by simply considering four of them. Although we need to evaluate the integral by summation of those from $-\infty$ to $-V/2$ and from $-V/2$ to E_F, since all the Green's functions are the same, we can take it directly from $-\infty$ to E_F.

$$\chi = -\frac{2}{\pi} Im \int_{-\infty}^{E_F} dE \quad 4G_K^{AA}(\mathbf{x} > 0, \mathbf{x}' < 0) G_K^{AA}(\mathbf{x}' < 0, \mathbf{x} > 0) \tag{2.60}$$

$$= Im \int_{-\infty}^{E_F} dE \quad \frac{i\left(E^2 - \frac{V^2}{4}\right) e^{2i\left(\frac{\left(E-\frac{V}{2}\right)}{\hbar v_F}x - \frac{\left(E+\frac{V}{2}\right)}{\hbar v_F}x'\right)}}{\hbar^3 v_F^3 \left(E(x-x') + \frac{V}{2}(x+x')\right)} \tag{2.61}$$

Result contains exponential integral and can be seen as

$$\chi = Im \left[\frac{ie^{-2iV(x+x')} \left(e^{i((2E(x-x')+V(x+x'))))} \left(1 - 2iE(x-x') + iV(x+x')\right)\right)}{8\hbar^3 v_F^3 (x-x')^3} + \frac{ie^{-2iV(x+x')} \left(4V^2 x x' \mathrm{Ei}\left(i(2E(x-x') + V(x+x'))\right)\right)}{8\hbar^3 v_F^3 (x-x')^3} \right]_{-\infty}^{E_F} \tag{2.62}$$

where the exponential integral is defined as

$$Ei(\xi) = \int_{-\infty}^{\xi} \frac{e^{\mu}}{\mu} d\mu \tag{2.63}$$

When we look at graphs (fig. 2.3 to fig. 2.8), susceptibility we found is as expected. Our results are supported by literature (Cheianov et al. (2007); Reijnders and Katsnelson (2017a); Reijnders and Katsnelson (2017b)) .When the receiver position is symmetrical to the source position and $E_F = 0$ focusing effect is strongly felt. By changing Fermi energy, effect is getting weaker but still focusing occurs. By interchanging the positions of the source and receiver, similar effect can be seen. Fig 2.9 and 2.10 shows the focusing effect with respect to Fermi energy when the position of the source is changing. On fig 2.11 and 2.12, the contribution with various position and Fermi energy values to the susceptibility can be seen.

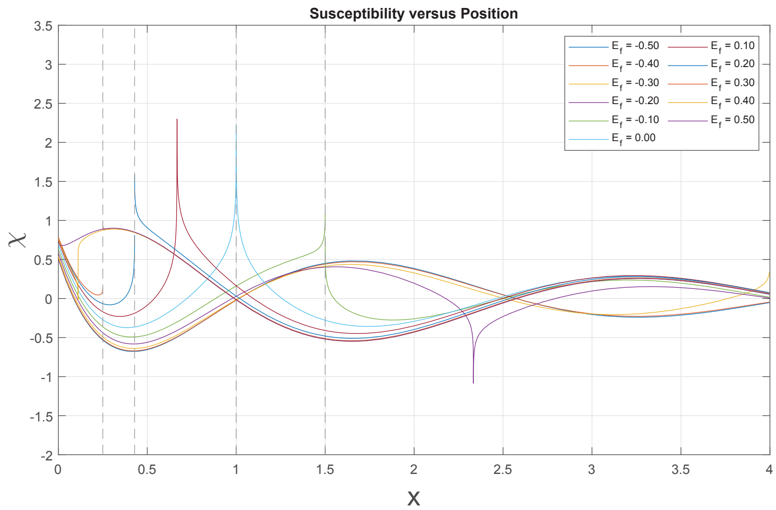


Figure 2.3. Graph shows susceptibility with respect to position (index in the x-axis is changed from $\overline{x}$ to x) with various E_F values. Strongest contribution is at $x = 1$ when the source is at $x' = -1$. Scaling is as follows: $l = \hbar v_F / V$, $\overline{E} = E/V$, $\overline{x} = xV/\hbar v_F$, $\overline{x}' = x'V/\hbar v_F$

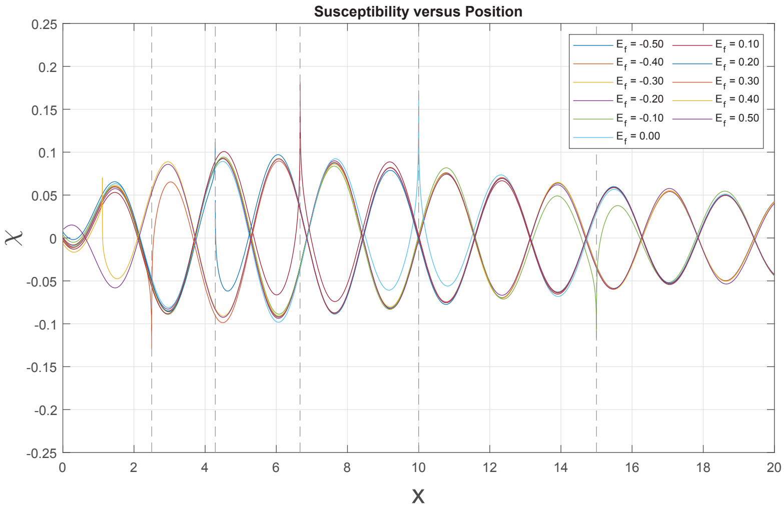


Figure 2.4. Graph shows susceptibility with respect to position (index in the x-axis is changed from $\overline{x}$ to x) with various E_F values. Strongest contribution is at $x = 10$ when the source is at $x' = -10$. Scaling is as follows: $l = \hbar v_F/V$, $\overline{E} = E/V$, $\overline{x} = xV/\hbar v_F$, $\overline{x}' = x'V/\hbar v_F$

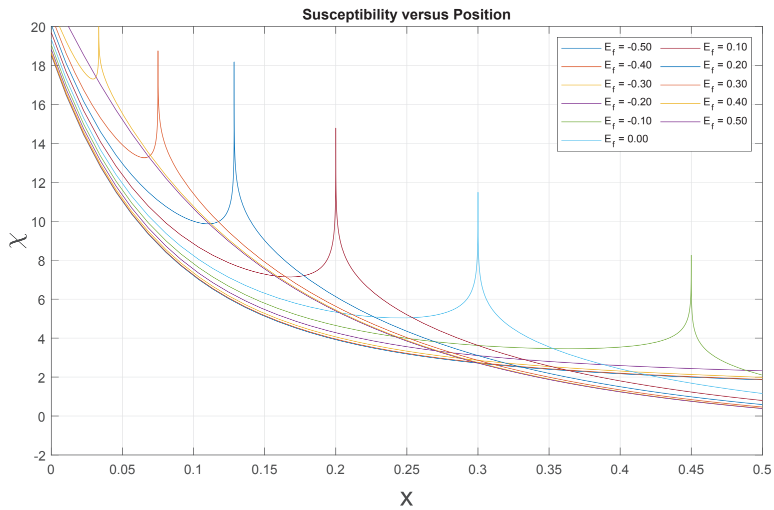


Figure 2.5. Graph shows susceptibility with respect to position (index in the x-axis is changed from $\overline{x}$ to x) with various E_F values. Strongest contribution is at $x = 0.3$ when the source is at $x' = -0.3$. Scaling is as follows: $l = \hbar v_F/V$, $\overline{E} = E/V$, $\overline{x} = xV/\hbar v_F$, $\overline{x}' = x'V/\hbar v_F$

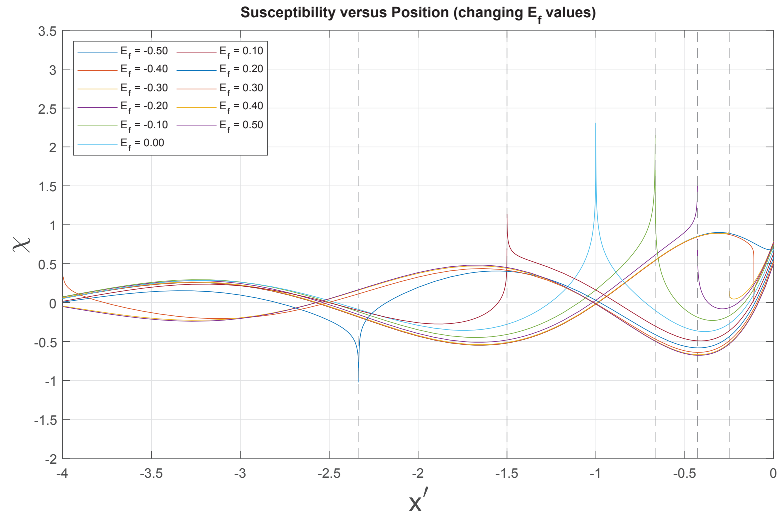


Figure 2.6. Graph shows susceptibility with respect to position (index in the x-axis is changed from $\overline{x}'$ to x') with various E_F values. Strongest contribution is at $x' = -1$ when the source is at $x = 1$. Scaling is as follows: $l = \hbar v_F/V$, $\overline{E} = E/V$, $\overline{x} = xV/\hbar v_F$, $\overline{x}' = x'V/\hbar v_F$

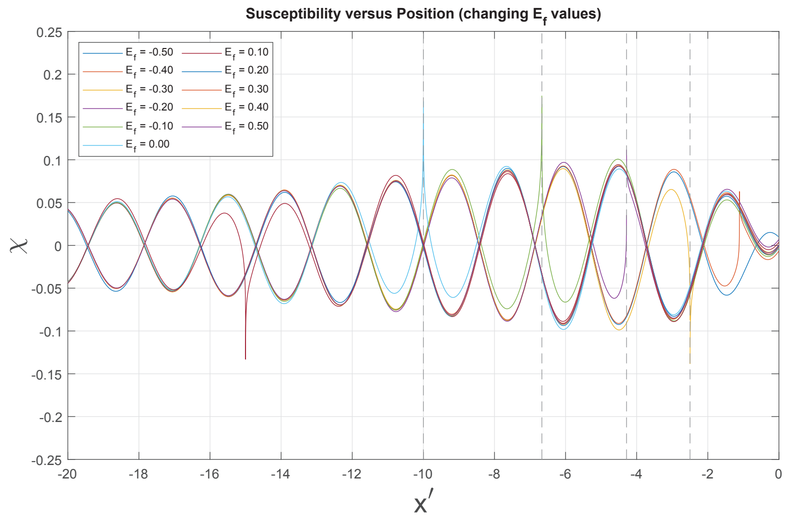


Figure 2.7. Graph shows susceptibility with respect to position (index in the x-axis is changed from $\overline{x}'$ to x') with various E_F values. Strongest contribution is at $x' = -10$ when the source is at $x = 10$. Scaling is as follows: $l = \hbar v_F/V$, $\overline{E} = E/V$, $\overline{x} = xV/\hbar v_F$, $\overline{x}' = x'V/\hbar v_F$

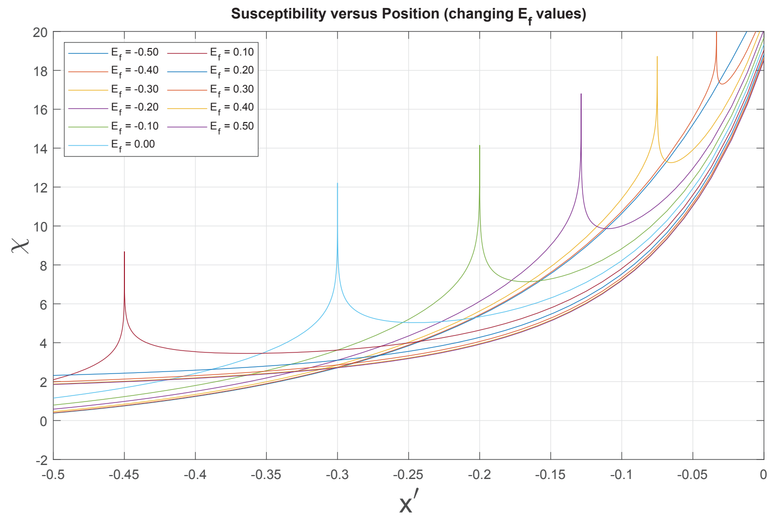


Figure 2.8. Graph shows susceptibility with respect to position (index in the x-axis is changed from $\overline{x}'$ to x') with various E_F values. Strongest contribution is at $x' = -0.3$ when the source is at $x = 0.3$. Scaling is as follows: $l = \hbar v_F/V, \overline{E} = E/V, \overline{x} = xV/\hbar v_F, \overline{x}' = x'V/\hbar v_F$

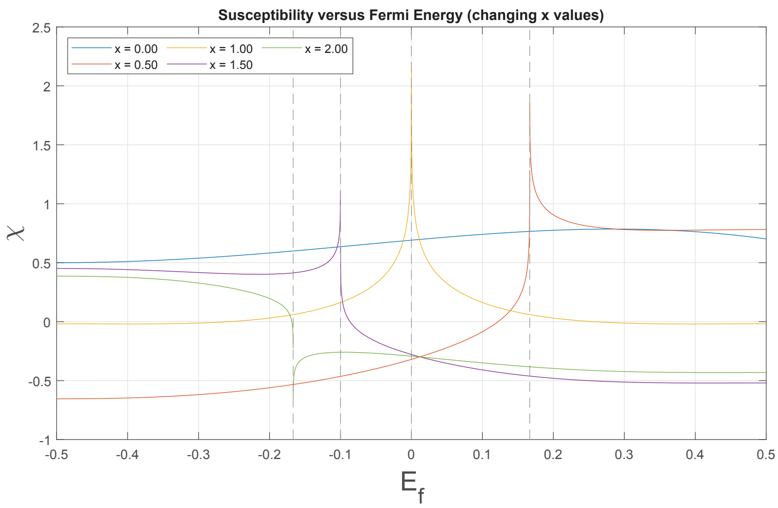


Figure 2.9. Graph shows susceptibility with respect to Fermi energy with various x values. Strongest contribution is at $E_F = 0$. Scaling is as follows: $l = \hbar v_F/V, \overline{E} = E/V, \overline{x} = xV/\hbar v_F, \overline{x}' = x'V/\hbar v_F$

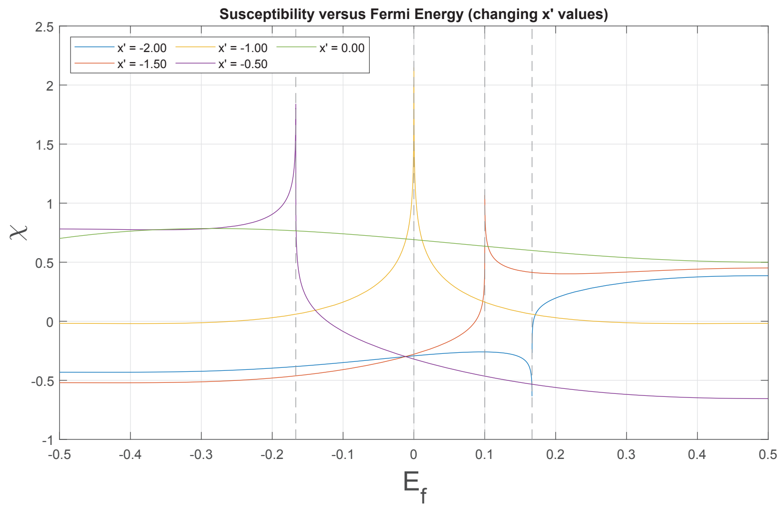


Figure 2.10. Graph shows susceptibility with respect to Fermi energy with various x' values. Strongest contribution is at $E_F = 0$. Scaling is as follows: $l = \hbar v_F/V$, $\overline{E} = E/V$, $\overline{x} = xV/\hbar v_F$, $\overline{x}' = x'V/\hbar v_F$

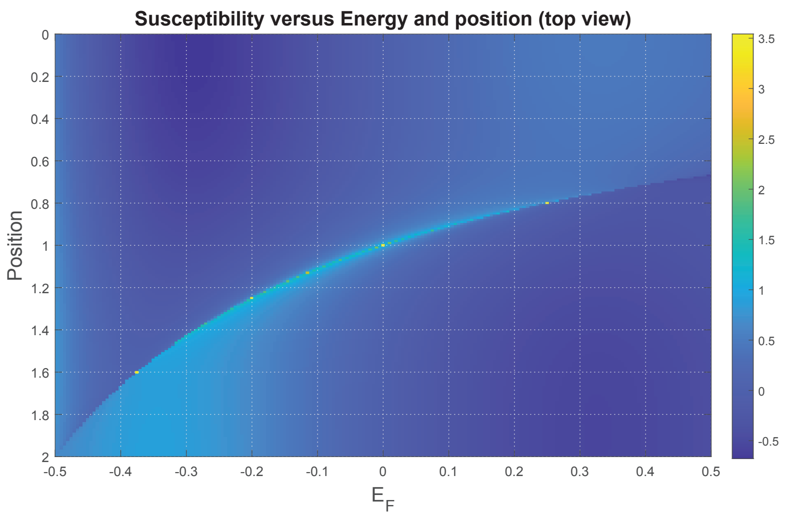


Figure 2.11. Graph shows susceptibility with respect to position and Fermi energy with various x and E_F values. When $x' = -1$, strongest contribution is at $E_F = 0$ and at $x = 1$. Scaling is as follows: $l = \hbar v_F/V$, $\overline{E} = E/V$, $\overline{x} = xV/\hbar v_F$, $\overline{x}' = x'V/\hbar v_F$

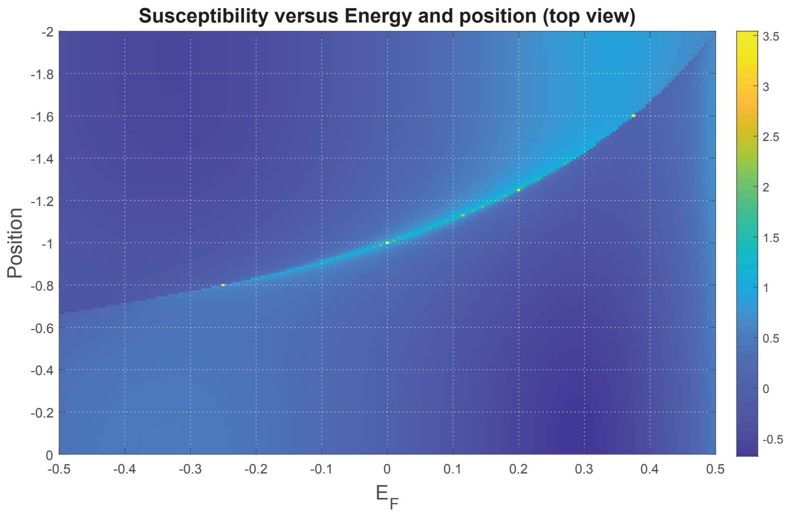


Figure 2.12. Graph shows susceptibility with respect to position and Fermi energy with various x' and E_F values. When $x = 1$, strongest contribution is at $E_F = 0$ and at $x' = -1$. Scaling is as follows: $l = \hbar v_F/V$, $\overline{E} = E/V$, $\overline{x} = xV/\hbar v_F$, $\overline{x}' = x'V/\hbar v_F$

CHAPTER 3

CONCLUSION

In this thesis, we have investigated the effect of Veselago lensing in graphene. To do this, we have considered n-p junction by considering a step potential barrier. We located two points for the source and the receiver on the opposite sides of the barrier. We also see the same effect by interchanging the positions of these two points. Due to the negative direction of the hole momentum with respect to incoming electron momentum, focusing effect occurs. After the analytical calculations, we found the Green's functions. Using the stationary phase approximation, we found the Green's functions around K and K' Dirac points. Because of the stationary phase approximation around $k = 0$ points, we had same AA(BB) components of the Green's functions for K and K' points. Unlike AA(BB) points, Green's functions for AB(BA) points are slightly different. However, we obtain the same susceptibility for both AA and AB points for symmetrically placed source and receiver. We have observed that perfect focusing occurs when the source and the receiver are equidistant from the barrier at zero Fermi energy. For a given receiver position, we determine the focusing point for various Fermi energies.

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APPENDIX A

EXPLICIT ANALYTICAL CALCULATIONS OF SUSCEPTIBILITY FOR GRAPHENE

In this chapter, Green's function calculations for our problem and that for bulk graphene are shown explicitly. Then, susceptibility, χ is computed from the derived Green's functions.

1) In cartesian coordinate, there is non-homogeneous differential equation needs to be solved.

$$(E - \hat{H}_K)G(\vec{r} - \vec{r}') = \delta(\vec{r} - \vec{r}') \tag{A.1}$$

Solution of the non-homogeneous differential equation is

$$G(\vec{r} - \vec{r}') = \begin{pmatrix} G^{AA} & G^{AB} \\ G^{BA} & G^{BB} \end{pmatrix} \tag{A.2}$$

Corresponding Hamiltonians for the K and K' points are

$$\hat{H}_K = V + v_F \vec{\sigma} \cdot \vec{p} \tag{A.3}$$

$$\hat{H}_{K'} = V + v_F \vec{\sigma}^* \cdot \vec{p} \tag{A.4}$$

$$\vec{\sigma} = (\sigma_x, \sigma_y) \tag{A.5}$$

$$\vec{\sigma}^* = (\sigma_x, -\sigma_y) \tag{A.6}$$

σ's are the Pauli matrices and p's are momentum operators.

$$\vec{\sigma} = \hat{\sigma}_x \hat{\imath} + \hat{\sigma}_y \hat{\jmath} \tag{A.7}$$

$$\vec{p} = \hat{p}_x \hat{\imath} + \hat{p}_y \hat{\jmath} \tag{A.8}$$

$$\hat{H}_K = \begin{pmatrix} V & v_F \hat{p}_- \\ v_F \hat{p}_+ & V \end{pmatrix} \tag{A.9}$$

where

$$\hat{p}_- = \hat{p}_x - i\hat{p}_y \tag{A.10}$$

$$\hat{p}_+ = \hat{p}_x + i\hat{p}_y \tag{A.11}$$

$$(E - \hat{H}_K) = \begin{pmatrix} E - V & -v_F \hat{p}_- \\ -v_F \hat{p}_+ & E - V \end{pmatrix} \tag{A.12}$$

$$\begin{pmatrix} E - V & -v_F \hat{p}_- \\ -v_F \hat{p}_+ & E - V \end{pmatrix} \begin{pmatrix} G^{AA} & G^{AB} \\ G^{BA} & G^{BB} \end{pmatrix} = \begin{pmatrix} \delta(\vec{r} - \vec{r}') & 0 \\ 0 & \delta(\vec{r} - \vec{r}') \end{pmatrix} \tag{A.13}$$

We have four equations for Green's Functions below

$$(E - V)G^{AA} - v_F \hat{p}_- G^{BA} = \delta(\vec{r} - \vec{r}') \tag{A.14}$$

$$(E - V)G^{AB} - v_F \hat{p}_- G^{BB} = 0 \tag{A.15}$$

$$-v_F \hat{p}_+ G^{AA} + (E - V)G^{BA} = 0 \tag{A.16}$$

$$-v_F \hat{p}_+ G^{AB} + (E - V)G^{BB} = \delta(\vec{r} - \vec{r}') \tag{A.17}$$

If we solve for G^{AA} we get

$$(E - V)G^{AA} - |v_F|^2 \hat{p}_- \frac{1}{(E - V)} \hat{p}_+ G^{AA} = \delta(\vec{r} - \vec{r}') \tag{A.18}$$

For Bulk graphene;

If there is no potential, $V = 0$, and we set for $v_F = 1$, then equation becomes

$$E^2 G^{AA} - (\hat{p}_x^2 + \hat{p}_y^2) G^{AA} = E\delta(\vec{r} - \vec{r}') \tag{A.19}$$

$$\frac{E^2}{\hbar^2} G^{AA} + \nabla^2 G^{AA} = \frac{E}{\hbar^2}\delta(\vec{r} - \vec{r}') \tag{A.20}$$

This (equation A.20) is well-known two-dimensional Helmholtz equation (Duffy (2015); Couto (2013))

$$E^2 G_{AA} - \hbar^2 (k_x^2 + k_y^2) G_{AA} = E\delta(\vec{r} - \vec{r}') \tag{A.21}$$

Taking the Fourier transformation of this equation gives

$$\frac{E^2}{\hbar^2} \bar{G}_{AA} - k^2 \bar{G}_{AA} = \frac{E}{\hbar^2} \frac{e^{i\vec{k}\cdot\vec{r}'}}{2\pi} \tag{A.22}$$

$$\bar{G}_{AA} = \frac{-E}{2\pi\hbar^2} \frac{e^{i\vec{k}\cdot\vec{r}'}}{\left(k^2 - \frac{E^2}{\hbar^2}\right)} \tag{A.23}$$

and then taking the inverse Fourier transformation gives

$$G_{AA} = \frac{-E}{\hbar^2} \frac{1}{(2\pi)^2} \int\limits_{\mathbb{R}^2} d^2k \frac{e^{-i\vec{k}\cdot\vec{R}}}{\left(k^2 - \frac{E^2}{\hbar^2}\right)} \tag{A.24}$$

where $\vec{R} \equiv \ (\vec{r} - \vec{r}')$

$$G_{AA} = -\frac{E}{(2\pi)^2 \hbar^2} \int\limits_{-\infty}^{\infty} dk_x e^{ik_x R} \int\limits_{-\infty}^{\infty} \frac{dk_y}{k_x^2 + k_y^2 - \frac{E^2}{\hbar^2}} \tag{A.25}$$

$$I = \int\limits_{-\infty}^{\infty} \frac{dk_y}{k_x^2 + k_y^2 - \frac{E^2}{\hbar^2}} \tag{A.26}$$

• for $|k_x| > \frac{E}{\hbar}$

$$k_y^2 + k_x^2 - \frac{E^2}{\hbar^2} = \left(k_y + i\sqrt{k_x^2 - \frac{E^2}{\hbar^2}}\right)\left(k_y - i\sqrt{k_x^2 - \frac{E^2}{\hbar^2}}\right) \tag{A.27}$$

There is only one pole inside the contour, which is $\left(i\sqrt{k_x^2 - \frac{E^2}{\hbar^2}}\right)$

$$I = 2\pi i Res\left(i\sqrt{k_x^2 - \frac{E^2}{\hbar^2}}\right) \tag{A.28}$$

$$= \frac{2\pi i}{2i\sqrt{k_x^2 - \frac{E^2}{\hbar^2}}} \tag{A.29}$$

$$= \frac{\pi}{\sqrt{k_x^2 - \frac{E^2}{\hbar^2}}} \tag{A.30}$$

• for $|k_x| < \frac{E}{\hbar}$

$$k_y^2 - \left(\frac{E^2}{\hbar^2} - k_x^2\right) = \left(k_y - \sqrt{\frac{E^2}{\hbar^2} - k_x}\right)\left(k_y + \sqrt{\frac{E^2}{\hbar^2} - k_x}\right) \tag{A.31}$$

$$\Rightarrow I = 2\pi i Res\left(\mp\sqrt{\frac{E^2}{\hbar^2} - k_x^2}\right) \tag{A.32}$$

$$= \mp\frac{2\pi i}{2\sqrt{\frac{E^2}{\hbar^2} - k_x^2}} \tag{A.33}$$

$$= \mp\frac{\pi i}{\sqrt{\frac{E^2}{\hbar^2} - k_x^2}} \tag{A.34}$$

$$G_{AA} = -\frac{E}{(2\pi)^2\hbar^2}\left[\pi\int_{-\infty}^{\infty}\frac{dk_x e^{ik_xR}}{\sqrt{k_x^2-\frac{E^2}{\hbar^2}}} \mp i\pi\int_{-\infty}^{\infty}\frac{dk_x e^{ik_xR}}{\sqrt{\frac{E^2}{\hbar^2}-k_x}}\right] \tag{A.35}$$

$$e^{ik_xR} \longrightarrow Cos(k_xR) + iSin(k_xR) \;(\to 0) \tag{A.36}$$

$$\Rightarrow G_{AA} = -\frac{E}{(2\pi)^2\hbar^2}\left[2\pi\underbrace{\int_{-\frac{E}{\hbar}}^{\infty}\frac{dk_x Cos(k_xR)}{\sqrt{k_x^2-\frac{E^2}{\hbar^2}}}}_{I_1} \mp 2i\pi\underbrace{\int_{0}^{\frac{E}{\hbar}}\frac{dk_x Cos(k_xR)}{\sqrt{\frac{E^2}{\hbar^2}-k_x^2}}}_{I_2}\right] \tag{A.37}$$

I_1	I_2
$k_x = \frac{E}{\hbar}u \quad \Rightarrow \quad dk_x = \frac{E}{\hbar}du$	$k_x = \frac{E}{\hbar}Cos\theta \quad \Rightarrow \quad dk_x = -\frac{E}{\hbar}Sin\theta d\theta$
$I_1 = \int_1^{\infty}\frac{\frac{E}{\hbar}Cos\left(\frac{E}{\hbar}uR\right)}{\sqrt{\frac{E^2}{\hbar^2}u^2-\frac{E^2}{\hbar^2}}}$	$I_2 = i\int_0^{\frac{\pi}{2}}\frac{-\frac{E}{\hbar}Sin\theta Cos\left(\frac{E}{\hbar}RCos\theta\right)d\theta}{\frac{E}{\hbar}\underbrace{\sqrt{1-Cos^2\theta}}_{Sin\theta}}$
$I_1 = \int_1^{\infty}\frac{Cos\left(\frac{E}{\hbar}uR\right)du}{\sqrt{u^2-1}}$	$I_2 = -i\int_0^{\frac{\pi}{2}}Cos\left(\frac{E}{\hbar}RCos\theta\right)d\theta$
$I_1 = -\frac{\pi}{2}N_0\left(\frac{E}{\hbar}R\right)$	$I_2 = -i\frac{\pi}{2}J_0\left(\frac{E}{\hbar}R\right)$

(A.38)

$$\Rightarrow G_{AA} = -\frac{E}{\hbar^2}\frac{1}{2\pi}\left(-\frac{\pi}{2}N_0\left(\frac{E}{\hbar}R\right) \pm i\frac{\pi}{2}J_0\left(\frac{E}{\hbar}R\right)\right) \tag{A.39}$$

$$= \frac{E}{4\hbar^2}\left(N_0\left(\frac{E}{\hbar}R\right) \pm iJ_0\left(\frac{E}{\hbar}R\right)\right) \tag{A.40}$$

$$= \frac{iE}{4\hbar^2}\left(J_0\left(\frac{ER}{\hbar}\right) \pm iN_0\left(\frac{ER}{\hbar}\right)\right) \tag{A.41}$$

$$= \pm\frac{E}{4\hbar^2}iH_0\left(\frac{ER}{\hbar}\right) \tag{A.42}$$

Plus sign is associated with the outgoing wave solution, that is why we need to pick that solution.

$$\Rightarrow \quad G_{AA} = \frac{E}{4\hbar^2} i H_0 \left(\frac{ER}{\hbar} \right) \tag{A.43}$$

from (A.15) and (A.16);

$$G_{AB} = \frac{-i\hbar \frac{\partial G_{BB}}{\partial x}}{E} \tag{A.44}$$

$$G_{BA} = \frac{-i\hbar \frac{\partial G_{AA}}{\partial x}}{E} \tag{A.45}$$

where

$$H_0^{'}(x) = -H_1(x) \tag{A.46}$$

$$G_{AA} = G_{BB} \tag{A.47}$$

$$G_{AB} = G_{BA}^{*} \tag{A.48}$$

$$\Rightarrow \qquad G_{BB} = \frac{E}{4\hbar^2} i H_0 \left(\frac{ER}{\hbar} \right) \tag{A.49}$$

$$G_{AB} = G_{BA} = -\frac{E}{4\hbar^2} H_1^{(1)} \left(\frac{ER}{\hbar} \right) \tag{A.50}$$

$$G = \begin{pmatrix} G_{AA} & G_{AB} \\ G_{BA} & G_{BB} \end{pmatrix} \tag{A.51}$$

$$\longrightarrow \boxed{G = \begin{pmatrix} \frac{E}{4\hbar^2} i H_0 \left(\frac{ER}{\hbar} \right) & -\frac{E}{4\hbar^2} H_1^{(1)} \left(\frac{ER}{\hbar} \right) \\ -\frac{E}{4\hbar^2} H_1^{(1)} \left(\frac{ER}{\hbar} \right) & \frac{E}{4\hbar^2} i H_0 \left(\frac{ER}{\hbar} \right) \end{pmatrix}} \tag{A.52}$$

2) In polar coordinate;

$$\left[E^2 + \hbar^2 \left(\underbrace{\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}}_{\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial}{\partial r})} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2} \right)\right] G = \frac{E}{r}\delta(r - r')\underbrace{\delta(\phi - \phi')}_{\frac{1}{2\pi}\sum e^{im\phi}} \tag{A.53}$$

$$\Rightarrow \frac{E^2}{\hbar^2}G_m + \frac{\partial^2 G_m}{\partial r^2} + \frac{1}{r}\frac{\partial G_m}{\partial r} - \frac{m^2}{r^2}G_m = \underbrace{\frac{E}{2\pi\hbar^2 r}\delta(r - r')}_{\frac{E}{2\pi\hbar^2 r'}} \tag{A.54}$$

$$G_m = \begin{cases} AJ_0\left(\frac{Er}{\hbar}\right), & 0 \le r \le r' \\ \\ BH_0^{(1)}\left(\frac{Er}{\hbar}\right), & r' \le r < \infty \end{cases} \tag{A.55}$$

i) $r = r'$

$$AJ_0\left(\frac{Er'}{\hbar}\right) = BH_0\left(\frac{Er'}{\hbar}\right) \tag{A.56}$$

$$\longrightarrow \quad \boxed{AJ_0\left(\frac{Er'}{\hbar}\right) - BH_0\left(\frac{Er'}{\hbar}\right) = 0} \tag{A.57}$$

ii) $\left(\frac{d}{dr}\right)\Big|_{r=r'^-}^{r=r'^+}$

$$r'\frac{dG_m}{dr}\Bigg|_{r=r'^-}^{r=r'^+} = \frac{E}{2\pi\hbar^2} \tag{A.58}$$

$$\frac{\not{E}}{\not{\hbar}}\left(BH_0'^{(1)}\left(\frac{Er'}{\hbar}\right) - AJ_0'\left(\frac{Er'}{\hbar}\right)\right) = \frac{\not{E}}{\not{\hbar}}\frac{1}{2\pi\hbar r'} \tag{A.59}$$

$$\Rightarrow \boxed{\left(-2\pi\hbar A J_0'\left(\frac{Er'}{\hbar}\right) + 2\pi\hbar B H_0'^{(1)}\left(\frac{Er'}{\hbar}\right)\right) = \frac{1}{r'}} \tag{A.60}$$

then we need to find constants in equation (A.57) and (A.60). To do this we need to find the Wronskian

$$\begin{pmatrix} J_0\left(\frac{Er'}{\hbar}\right) & -H_0^{(1)}\left(\frac{Er'}{\hbar}\right) \\ -2\pi\hbar J_0'\left(\frac{Er'}{\hbar}\right) & 2\pi\hbar H_0'^{(1)}\left(\frac{Er'}{\hbar}\right) \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{1}{r'} \end{pmatrix} \tag{A.61}$$

$$\Rightarrow \; W = -\tfrac{4i\hbar^2}{Er'} \tag{A.62}$$

$$A = \frac{\begin{vmatrix} 0 & -H_0^{(1)}\left(\frac{Er'}{\hbar}\right) \\ \frac{1}{r'} & 2\pi\hbar H_0'^{(1)}\left(\frac{Er'}{\hbar}\right) \end{vmatrix}}{W} = \frac{\frac{H_0^{(1)}}{r'}}{\frac{-4i\hbar^2}{Er'}} \tag{A.63}$$

$$A = \boxed{\frac{iEH_0^{(1)}}{4\hbar^2}} \tag{A.64}$$

$$B = \frac{\begin{vmatrix} J_0\left(\frac{Er'}{\hbar}\right) & 0 \\ 2\pi\hbar J_0'\left(\frac{Er'}{\hbar}\right) & \frac{1}{r'} \end{vmatrix}}{W} = \frac{\frac{J_0}{r'}}{-\frac{4i\hbar^2}{Er'}} \tag{A.65}$$

$$\Rightarrow B = \boxed{\frac{iEJ_0}{4\hbar^2}} \tag{A.66}$$

$$\Rightarrow \boxed{G_{AA} = \frac{iE}{4\hbar^2} \sum_{m=-\infty}^{\infty} J_m\left(\frac{Er_<}{\hbar}\right) H_m^{(1)}\left(\frac{Er_>}{\hbar}\right) e^{im\phi}} \tag{A.67}$$

For $v_f \neq 1$;

i) $x > 0, \quad x' < 0, \quad -\frac{V}{2} < E < \frac{V}{2}, \quad V > 0$

$$(E-V)G_K^{AA} - (-i\frac{\partial}{\partial x} - ik)\frac{\hbar^2 v_F^2}{(E-V)}(-i\frac{\partial}{\partial x} + ik)G_K^{AA} = \delta(x-x') \tag{A.68}$$

$$x > 0 \quad G_{K_1}^{AA} = Ae^{iqx} \tag{A.69}$$

$$x' < x < 0 \quad G_{K_2}^{AA} = Be^{iq'x} + Ce^{-iq'x} \tag{A.70}$$

$$x < x' < 0 \quad G_{K_3}^{AA} = De^{-iq'x} \tag{A.71}$$

Boundary conditions are;

$$(i) \quad x = x' \tag{A.72}$$

$$(ii) \quad \frac{\partial G_K^{AA}}{\partial x}\Bigg|_{x=x'-\epsilon}^{x=x'+\epsilon} = 1 \tag{A.73}$$

$$(iii) \quad x = 0 \tag{A.74}$$

$$(iv) \quad \frac{\partial G_K^{AA}}{\partial x}\Bigg|_{x=0-\epsilon}^{x=0+\epsilon} = 0 \tag{A.75}$$

There is a discontinuity at $x = 0$ and potentials, V_i's on each side are; $V_{left} = -V/2$ for $x < 0$ (when $i =$ left), $V_{right} = V/2$ for $x > 0$ (when $i =$ right)

$$(i) \quad G_{K_2}^{AA}\Bigg|_{x=x'} = G_{K_3}^{AA}\Bigg|_{x=x'} \tag{A.76}$$

$$\Rightarrow \quad Be^{iq'x'} + Ce^{-iq'x'} = De^{-iq'x'} \tag{A.77}$$

$$\Rightarrow \quad Be^{iq'x'} + Ce^{-iq'x'} - De^{-iq'x'} = 0 \tag{A.78}$$

$$(ii) \quad \left(\frac{\hbar^2 v_F^2}{(E-V_i)}\right)\left(\frac{\partial G_K^{AA}}{\partial x}\Bigg|_{x=x'-\epsilon}^{x=x'+\epsilon} - kG_K^{AA}\Bigg|_{x=x'-\epsilon}^{x=x'+\epsilon}\right) = 1 \tag{A.79}$$

$$\Rightarrow \quad \left(\frac{\hbar^2 v_F^2}{(E+\frac{V}{2})}\right)\Big[(iq'-k)Be^{iq'x'} + (-iq'-k)Ce^{-iq'x'} - (-iq'-k)De^{-iq'x'}\Big] = 1 \tag{A.80}$$

$$\Rightarrow \quad -(k-iq')Be^{iq'x'} - (k+iq')Ce^{-iq'x'} + (k+iq')De^{-iq'x'} = \frac{(E+\frac{V}{2})}{\hbar^2 v_F^2} \tag{A.81}$$

$$(iii) \quad x = 0 \tag{A.82}$$

$$\Rightarrow \quad A = B + C \tag{A.83}$$

$$\Rightarrow \quad A - B - C = 0 \tag{A.84}$$

$$(iv) \quad \left(\frac{\hbar^2 v_F^2}{(E-V_i)}\right)\left(\frac{\partial G_K^{AA}}{\partial x}\Bigg|_{x=0-\epsilon}^{x=0+\epsilon} - kG_K^{AA}\Bigg|_{x=0-\epsilon}^{x=0+\epsilon}\right) = 0 \tag{A.85}$$

$$\Rightarrow \quad \frac{\hbar^2 v_F^2}{(E-\frac{V}{2})}(iq-k)A - \frac{\hbar^2 v_F^2}{(E+\frac{V}{2})}((iq'-k)B + (-iq'-k)C) = 0 \tag{A.86}$$

$$\Rightarrow \quad -\frac{\hbar^2 v_F^2(k-iq)}{(E-\frac{V}{2})}A + \frac{\hbar^2 v_F^2(k-iq')}{(E+\frac{V}{2})}B + \frac{\hbar^2 v_F^2(k+iq')}{(E+\frac{V}{2})}C = 0 \tag{A.87}$$

After some algebra, G_K^{AA} can be found as;

$$G_K^{AA} = \frac{(E^2 - \frac{V^2}{4})}{\hbar^2 v_F^2(-kV + iE(q+q') + i\frac{V}{2}(q-q'))} \quad e^{iqx - iq'x'} \tag{A.88}$$

$$G_{K'}^{AA} = \frac{(E^2 - \frac{V^2}{4})}{\hbar^2 v_F^2(kV + iE(q+q') + i\frac{V}{2}(q-q'))} \quad e^{iqx - iq'x'} \tag{A.89}$$

Where;

$$q = -\sqrt{\frac{\left(E - \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2} \tag{A.90}$$

$$q' = \sqrt{\frac{\left(E + \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2} \tag{A.91}$$

To find Green's function, stationary phase approximation method is used around $k = 0$ point.

$$S = -\left(\sqrt{\frac{\left(E - \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2}\right) x - \left(\sqrt{\frac{\left(E + \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2}\right) x' \tag{A.92}$$

$$\frac{\partial S}{\partial k} = \frac{xk}{\left(\frac{\left(E - \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2\right)^{1/2}} + \frac{x'k}{\left(\frac{\left(E + \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2\right)^{1/2}} \tag{A.93}$$

$$\frac{\partial^2 S}{\partial k^2} = \frac{x\frac{\left(E - \frac{V}{2}\right)^2}{\hbar^2 v_F^2}}{\left(\frac{\left(E - \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2\right)^{3/2}} + \frac{x'\frac{\left(E + \frac{V}{2}\right)^2}{\hbar^2 v_F^2}}{\left(\frac{\left(E + \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2\right)^{3/2}} \tag{A.94}$$

$$S \approx -\sqrt{\frac{\left(E - \frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x - \sqrt{\frac{\left(E + \frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x' + \frac{1}{2}\frac{xk^2}{\sqrt{\frac{\left(E - \frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} + \frac{1}{2}\frac{x'k^2}{\sqrt{\frac{\left(E + \frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} \tag{A.95}$$

$$\int dk \quad e^{iS} f(k) = e^{iS_0} \quad \sqrt{\frac{i\pi}{S_2}} \quad f(k(x,y)) \tag{A.96}$$

$$\Rightarrow G_K^{AA}(\mathbf{x} > 0, \mathbf{x}' < 0) = \int dk \quad e^{iS} G_K^{AA} \tag{A.97}$$

where S_0 and S_2 are;

$$S_0 = -\sqrt{\frac{\left(E - \frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x - \sqrt{\frac{\left(E + \frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x' \tag{A.98}$$

$$S_2 = \frac{1}{2}\frac{xk^2}{\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} + \frac{1}{2}\frac{x'k^2}{\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} \tag{A.99}$$

$$G_K^{AA}(\mathbf{x} > 0, \mathbf{x}' < 0) = \frac{\left(E^2 - \frac{V^2}{4}\right) e^{i\left(-\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x - \sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x'\right)} \sqrt{\frac{2i\pi}{\frac{x}{\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} + \frac{x'}{\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}}}}}{\hbar^2 v_F^2 \left((-iE - i\frac{V}{2})\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} + (iE - i\frac{V}{2})\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} \right)} \tag{A.100}$$

$$G_{K'}^{AA}(\mathbf{x} > 0, \mathbf{x}' < 0) = \frac{\left(E^2 - \frac{V^2}{4}\right) e^{i\left(-\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x - \sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x'\right)} \sqrt{\frac{2i\pi}{\frac{x}{\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} + \frac{x'}{\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}}}}}{\hbar^2 v_F^2 \left((-iE - i\frac{V}{2})\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} + (iE - i\frac{V}{2})\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} \right)} \tag{A.101}$$

ii) $x < 0, \quad x' > 0, \quad -\frac{V}{2} < E < \frac{V}{2}, \quad V > 0$

$$x > x' > 0 \quad G'^{AA}_{K_1} = Ae^{iqx} \tag{A.102}$$

$$x' > x > 0 \quad G'^{AA}_{K_2} = Be^{iqx} + Ce^{-iqx} \tag{A.103}$$

$$x < 0 \quad G'^{AA}_{K_3} = De^{-iq'x} \tag{A.104}$$

Boundary conditions are;

$$(i) \quad x = x' \tag{A.105}$$

$$(ii) \quad \frac{\partial G'^{AA}_{K}}{\partial x}\bigg|_{x=x'-\epsilon}^{x=x'+\epsilon} = 1 \tag{A.106}$$

$$(iii) \quad x = 0 \tag{A.107}$$

$$(iv) \quad \frac{\partial G'^{AA}_{K}}{\partial x}\bigg|_{x=0-\epsilon}^{x=0+\epsilon} = 0 \tag{A.108}$$

$$(i) \quad G'^{AA}_{K_1}\bigg|_{x=x'} = G'^{AA}_{K_2}\bigg|_{x=x'} \tag{A.109}$$

$$\Rightarrow \quad Ae^{iqx'} = Be^{iqx'} + Ce^{-iqx'} \tag{A.110}$$

$$\Rightarrow \quad Ae^{iqx'} - Be^{iqx'} - Ce^{-iqx'} = 0 \tag{A.111}$$

$$(ii) \quad \left(\frac{\hbar^2 v_F^2}{(E-V_i)}\right)\left(\frac{\partial G_K'^{AA}}{\partial x}\Bigg|_{x=x'-\epsilon}^{x=x'+\epsilon} - kG_K'^{AA}\Bigg|_{x=x'-\epsilon}^{x=x'+\epsilon}\right) = 1 \tag{A.112}$$

$$\Rightarrow \quad \left(\frac{\hbar^2 v_F^2}{(E-\frac{V}{2})}\right)\left[(iq-k)Ae^{iqx'} - (iq-k)Be^{iqx'} - (-iq-k)Ce^{-iqx'}\right] = 1 \tag{A.113}$$

$$\Rightarrow \quad -(k-iq)Ae^{iqx'} + (k-iq)Be^{iqx'} + (k+iq)Ce^{-iqx'} = \frac{(E-\frac{V}{2})}{\hbar^2 v_F^2} \tag{A.114}$$

$$(iii) \quad x = 0 \tag{A.115}$$

$$\Rightarrow \quad B + C = D \tag{A.116}$$

$$\Rightarrow \quad D - B - C = 0 \tag{A.117}$$

$$(iv) \quad \left(\frac{\hbar^2 v_F^2}{(E-V_i)}\right)\left(\frac{\partial G_K'^{AA}}{\partial x}\Bigg|_{x=0-\epsilon}^{x=0+\epsilon} - kG_K'^{AA}\Bigg|_{x=0-\epsilon}^{x=0+\epsilon}\right) = 0 \tag{A.118}$$

$$\Rightarrow \quad \frac{\hbar^2 v_F^2}{(E-\frac{V}{2})}((iq-k)B + (-iq-k)C) - \frac{\hbar^2 v_F^2}{(E+\frac{V}{2})}(-iq'-k)D = 0 \tag{A.119}$$

$$\Rightarrow \quad -\frac{\hbar^2 v_F^2(k-iq)}{(E-\frac{V}{2})}B - \frac{\hbar^2 v_F^2(k+iq)}{(E-\frac{V}{2})}C + \frac{\hbar^2 v_F^2(k+iq')}{(E+\frac{V}{2})}D = 0 \tag{A.120}$$

After some algebra, $G_K'^{AA}$ can be found as;

$$G_K'^{AA} = \frac{(E^2 - \frac{V^2}{4})}{\hbar^2 v_F^2(-kV + iE(q+q') + i\frac{V}{2}(q-q'))} \quad e^{iqx'-iq'x} \tag{A.121}$$

$$G_{K'}'^{AA} = \frac{(E^2 - \frac{V^2}{4})}{\hbar^2 v_F^2(kV + iE(q+q') + i\frac{V}{2}(q-q'))} \quad e^{iqx'-iq'x} \tag{A.122}$$

Where;

$$q = -\sqrt{\frac{\left(E - \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2} \tag{A.123}$$

$$q' = \sqrt{\frac{\left(E + \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2} \tag{A.124}$$

$$G_K^{AA}(\mathbf{x'} < 0, \mathbf{x} > 0) = \frac{\left(E^2 - \frac{V^2}{4}\right) e^{i\left(-\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x - \sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x'\right)} \sqrt{\frac{2i\pi}{\frac{x}{\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} + \frac{x'}{\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}}}}}{\hbar^2 v_F^2 \left((-iE - i\frac{V}{2})\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} + (iE - i\frac{V}{2})\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}\right)} \tag{A.125}$$

$$G_{K'}^{AA}(\mathbf{x'} < 0, \mathbf{x} > 0) = \frac{\left(E^2 - \frac{V^2}{4}\right) e^{i\left(-\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x - \sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x'\right)} \sqrt{\frac{2i\pi}{\frac{x}{\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} + \frac{x'}{\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}}}}}{\hbar^2 v_F^2 \left((-iE - i\frac{V}{2})\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} + (iE - i\frac{V}{2})\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}\right)} \tag{A.126}$$

$$\chi = -\frac{2}{\pi} Im \int_{-\frac{V}{2}}^{E_F} dE \quad G_K^{AA}(\mathbf{x} > 0, \mathbf{x}' < 0) G_K^{AA}(\mathbf{x}' < 0, \mathbf{x} > 0) \tag{A.127}$$

$$= Im \int_{-\frac{V}{2}}^{E_F} dE \quad \frac{i\left(E^2 - \frac{V^2}{4}\right) e^{2i\left(\frac{\left(E-\frac{V}{2}\right)}{\hbar v_F} x - \frac{\left(E+\frac{V}{2}\right)}{\hbar v_F} x'\right)}}{\hbar^3 v_F^3 \left(E(x-x') + \frac{V}{2}(x+x')\right)} \tag{A.128}$$

$$\chi = \left[\frac{i e^{-2iV(x+x')} \left(e^{i((2E(x-x')+V(x+x')))} \left(1 - 2iE(x-x') + iV(x+x')\right)\right)}{8\hbar^3 v_F^3 (x-x')^3} + \frac{i e^{-2iV(x+x')} \left(4V^2 x x' \mathrm{Ei}\left(i(2E(x-x') + V(x+x'))\right)\right)}{8\hbar^3 v_F^3 (x-x')^3} \right]_{-\frac{V}{2}}^{E_F} \tag{A.129}$$

For $v_f \neq 1$;

i) $x > 0, \quad x' < 0, \quad -\infty < E < -\frac{V}{2}, \quad V > 0$

$$(E-V) G_K^{AA} - (-i\frac{\partial}{\partial x} - ik) \frac{\hbar^2 v_F^2}{(E-V)} (-i\frac{\partial}{\partial x} + ik) G_K^{AA} = \delta(x - x') \tag{A.130}$$

$$x > 0 \quad G_{K_1}^{AA} = A e^{iqx} \tag{A.131}$$

$$x' < x < 0 \quad G_{K_2}^{AA} = B e^{iq'x} + C e^{-iq'x} \tag{A.132}$$

$$x < x' < 0 \quad G_{K_3}^{AA} = D e^{-iq'x} \tag{A.133}$$

Boundary conditions are;

$$(i) \quad x = x' \tag{A.134}$$

$$(ii) \quad \frac{\partial G_K^{AA}}{\partial x}\Bigg|_{x=x'-\epsilon}^{x=x'+\epsilon} = 1 \tag{A.135}$$

$$(iii) \quad x = 0 \tag{A.136}$$

$$(iv) \quad \frac{\partial G_K^{AA}}{\partial x}\Bigg|_{x=0-\epsilon}^{x=0+\epsilon} = 0 \tag{A.137}$$

There is a discontinuity at $x = 0$ and potentials, V_i's on each side are; $V_{left} = -V/2$ for $x < 0$ (when $i =$ left), $V_{right} = V/2$ for $x > 0$ (when $i =$ right)

$$(i) \quad G_{K_2}^{AA}\Bigg|_{x=x'} = G_{K_3}^{AA}\Bigg|_{x=x'} \tag{A.138}$$

$$\Rightarrow \quad Be^{iq'x'} + Ce^{-iq'x'} = De^{-iq'x'} \tag{A.139}$$

$$\Rightarrow \quad Be^{iq'x'} + Ce^{-iq'x'} - De^{-iq'x'} = 0 \tag{A.140}$$

$$(ii) \quad \left(\frac{\hbar^2 v_F^2}{(E - V_i)}\right)\left(\frac{\partial G_K^{AA}}{\partial x}\Bigg|_{x=x'-\epsilon}^{x=x'+\epsilon} - kG_K^{AA}\Bigg|_{x=x'-\epsilon}^{x=x'+\epsilon}\right) = 1 \tag{A.141}$$

$$\Rightarrow \quad \left(\frac{\hbar^2 v_F^2}{(E + \frac{V}{2})}\right)\left[(iq' - k)Be^{iq'x'} + (-iq' - k)Ce^{-iq'x'} - (-iq' - k)De^{-iq'x'}\right] = 1 \tag{A.142}$$

$$\Rightarrow \quad -(k-iq')Be^{iq'x'} - (k+iq')Ce^{-iq'x'} + (k+iq')De^{-iq'x'} = \frac{(E+\frac{V}{2})}{\hbar^2 v_F^2} \tag{A.143}$$

$$(iii) \quad x = 0 \tag{A.144}$$

$$\Rightarrow \quad A = B + C \tag{A.145}$$

$$\Rightarrow \quad A - B - C = 0 \tag{A.146}$$

$$(iv) \quad \left(\frac{\hbar^2 v_F^2}{(E-V_i)}\right)\left(\frac{\partial G_K^{AA}}{\partial x}\bigg|_{x=0-\epsilon}^{x=0+\epsilon} - kG_K^{AA}\bigg|_{x=0-\epsilon}^{x=0+\epsilon}\right) = 0 \tag{A.147}$$

$$\Rightarrow \quad \frac{\hbar^2 v_F^2}{(E-\frac{V}{2})}(iq-k)A - \frac{\hbar^2 v_F^2}{(E+\frac{V}{2})}((iq'-k)B + (-iq'-k)C) = 0 \tag{A.148}$$

$$\Rightarrow \quad -\frac{\hbar^2 v_F^2(k-iq)}{(E-\frac{V}{2})}A + \frac{\hbar^2 v_F^2(k-iq')}{(E+\frac{V}{2})}B + \frac{\hbar^2 v_F^2(k+iq')}{(E+\frac{V}{2})}C = 0 \tag{A.149}$$

After some algebra, G_K^{AA} can be found as;

$$G_K^{AA} = \frac{(E^2 - \frac{V^2}{4})}{\hbar^2 v_F^2(-kV + iE(q+q') + i\frac{V}{2}(q-q'))} \quad e^{iqx-iq'x'} \tag{A.150}$$

$$G_{K'}^{AA} = \frac{(E^2 - \frac{V^2}{4})}{\hbar^2 v_F^2(kV + iE(q+q') + i\frac{V}{2}(q-q'))} \quad e^{iqx-iq'x'} \tag{A.151}$$

Where;

$$\hat{H}_{K'} = v_F \vec{\sigma}^* \cdot \vec{p} \tag{A.152}$$

$$\vec{\sigma}^* = (\sigma_x, -\sigma_y) \tag{A.153}$$

$$q = -\sqrt{\frac{\left(E - \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2} \tag{A.154}$$

$$q' = -\sqrt{\frac{\left(E + \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2} \tag{A.155}$$

$$S = -\left(\sqrt{\frac{\left(E - \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2}\right) x + \left(\sqrt{\frac{\left(E + \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2}\right) x' \tag{A.156}$$

$$\frac{\partial S}{\partial k} = \frac{xk}{\left(\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2\right)^{1/2}} - \frac{x'k}{\left(\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2\right)^{1/2}} \tag{A.157}$$

$$\frac{\partial^2 S}{\partial k^2} = \frac{x\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}{\left(\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2\right)^{3/2}} - \frac{x'\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}{\left(\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2\right)^{3/2}} \tag{A.158}$$

$$S \approx -\sqrt{\frac{\left(E - \frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x + \sqrt{\frac{\left(E + \frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x' + \frac{1}{2}\frac{xk^2}{\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} - \frac{1}{2}\frac{x'k^2}{\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} \tag{A.159}$$

$$\int dk \quad e^{iS} f(k) = e^{iS_0} \quad \sqrt{\frac{i\pi}{S_2}} \quad f(k(x,y)) \tag{A.160}$$

$$\Rightarrow G_K^{AA}(\mathbf{x} > 0, \mathbf{x}' < 0) = \int dk \quad e^{iS} G_K^{AA} \tag{A.161}$$

$$G_K^{AA}(\mathbf{x} > 0, \mathbf{x}' < 0) = \frac{\left(E^2 - \frac{V^2}{4}\right) e^{i\left(-\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x + \sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x'\right)} \sqrt{\frac{2i\pi}{\frac{x}{\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} - \frac{x'}{\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}}}}}{\hbar^2 v_F^2 \left((-iE - i\frac{V}{2})\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} + (-iE + i\frac{V}{2})\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} \right)} \tag{A.162}$$

$$G_{K'}^{AA}(\mathbf{x} > 0, \mathbf{x}' < 0) = \frac{\left(E^2 - \frac{V^2}{4}\right) e^{i\left(-\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x + \sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x'\right)} \sqrt{\frac{2i\pi}{\frac{x}{\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} - \frac{x'}{\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}}}}}{\hbar^2 v_F^2 \left((-iE - i\frac{V}{2})\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} + (-iE + i\frac{V}{2})\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} \right)} \tag{A.163}$$

ii) $x < 0, \quad x' > 0, \quad -\infty < E < -\frac{V}{2}, \quad V > 0$

$$x > x' > 0 \quad G'^{AA}_{K_1} = Ae^{iqx} \tag{A.164}$$

$$x' > x > 0 \quad G'^{AA}_{K_2} = Be^{iqx} + Ce^{-iqx} \tag{A.165}$$

$$x < 0 \quad G'^{AA}_{K_3} = De^{-iq'x} \tag{A.166}$$

Boundary conditions are;

$$(i) \quad x = x' \tag{A.167}$$

$$(ii) \quad \frac{\partial G'^{AA}_K}{\partial x}\Bigg|_{x=x'-\epsilon}^{x=x'+\epsilon} = 1 \tag{A.168}$$

$$(iii) \quad x = 0 \tag{A.169}$$

$$(iv) \quad \frac{\partial G'^{AA}_K}{\partial x}\Bigg|_{x=0-\epsilon}^{x=0+\epsilon} = 0 \tag{A.170}$$

$$(i) \quad G'^{AA}_{K_1}\Bigg|_{x=x'} = G'^{AA}_{K_2}\Bigg|_{x=x'} \tag{A.171}$$

$$\Rightarrow \quad Ae^{iqx'} = Be^{iqx'} + Ce^{-iqx'} \tag{A.172}$$

$$\Rightarrow \quad Ae^{iqx'} - Be^{iqx'} - Ce^{-iqx'} = 0 \tag{A.173}$$

$$(ii) \quad \left(\frac{\hbar^2 v_F^2}{(E - V_i)}\right)\left(\frac{\partial G'^{AA}_K}{\partial x}\Bigg|_{x=x'-\epsilon}^{x=x'+\epsilon} - kG'^{AA}_K\Bigg|_{x=x'-\epsilon}^{x=x'+\epsilon}\right) = 1 \tag{A.174}$$

$$\Rightarrow \quad \left(\frac{\hbar^2 v_F^2}{(E - \frac{V}{2})}\right)\left[(iq-k)Ae^{iqx'} - (iq-k)Be^{iqx'} - (-iq-k)Ce^{-iqx'}\right] = 1 \tag{A.175}$$

$$\Rightarrow \quad -(k-iq)Ae^{iqx'} + (k-iq)Be^{iqx'} + (k+iq)Ce^{-iqx'} = \frac{(E-\frac{V}{2})}{\hbar^2 v_F^2} \tag{A.176}$$

$$(iii) \quad x = 0 \tag{A.177}$$

$$\Rightarrow \quad B + C = D \tag{A.178}$$

$$\Rightarrow \quad D - B - C = 0 \tag{A.179}$$

$$(iv) \quad \left(\frac{\hbar^2 v_F^2}{(E - V_i)}\right)\left(\frac{\partial G_K'^{AA}}{\partial x}\Bigg|_{x=0-\epsilon}^{x=0+\epsilon} - kG_K'^{AA}\Bigg|_{x=0-\epsilon}^{x=0+\epsilon}\right) = 0 \tag{A.180}$$

$$\Rightarrow \quad \frac{\hbar^2 v_F^2}{(E - \frac{V}{2})}((iq - k)B + (-iq - k)C) - \frac{\hbar^2 v_F^2}{(E + \frac{V}{2})}(-iq' - k)D = 0 \tag{A.181}$$

$$\Rightarrow \quad -\frac{\hbar^2 v_F^2 (k - iq)}{(E - \frac{V}{2})}B - \frac{\hbar^2 v_F^2 (k + iq)}{(E - \frac{V}{2})}C + \frac{\hbar^2 v_F^2 (k + iq')}{(E + \frac{V}{2})}D = 0 \tag{A.182}$$

After some algebra, $G_K'^{AA}$ can be found as;

$$G_K'^{AA} = \frac{(E^2 - \frac{V^2}{4})}{\hbar^2 v_F^2(-kV + iE(q + q') + i\frac{V}{2}(q - q'))} \quad e^{iqx' - iq'x} \tag{A.183}$$

$$G_{K'}'^{AA} = \frac{(E^2 - \frac{V^2}{4})}{\hbar^2 v_F^2(kV + iE(q + q') + i\frac{V}{2}(q - q'))} \quad e^{iqx' - iq'x} \tag{A.184}$$

Where;

$$q = -\sqrt{\frac{\left(E - \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2} \tag{A.185}$$

$$q' = -\sqrt{\frac{\left(E + \frac{V}{2}\right)^2}{\hbar^2 v_F^2} - k^2} \tag{A.186}$$

$$G_K^{AA}(\mathbf{x}' < 0, \mathbf{x} > 0) = \frac{\left(E^2 - \frac{V^2}{4}\right) e^{i\left(\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x - \sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x'\right)} \sqrt{\frac{2i\pi}{-\frac{x}{\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} + \frac{x'}{\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}}}}}{\hbar^2 v_F^2 \left((-iE - i\frac{V}{2})\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} + (-iE + i\frac{V}{2})\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}\right)} \tag{A.187}$$

$$G_{K'}^{AA}(\mathbf{x}' < 0, \mathbf{x} > 0) = \frac{\left(E^2 - \frac{V^2}{4}\right) e^{i\left(\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x - \sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}x'\right)} \sqrt{\frac{2i\pi}{-\frac{x}{\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}} + \frac{x'}{\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}}}}}{\hbar^2 v_F^2 \left((-iE - i\frac{V}{2})\sqrt{\frac{\left(E-\frac{V}{2}\right)^2}{\hbar^2 v_F^2}} + (-iE + i\frac{V}{2})\sqrt{\frac{\left(E+\frac{V}{2}\right)^2}{\hbar^2 v_F^2}}\right)} \tag{A.188}$$

$$\chi = -\frac{2}{\pi} Im \int_{-\infty}^{-\frac{V}{2}} dE \quad G_K^{AA}(\mathbf{x} > 0, \mathbf{x}' < 0) G_K^{AA}(\mathbf{x}' < 0, \mathbf{x} > 0) \tag{A.189}$$

$$= Im \int_{-\infty}^{-\frac{V}{2}} dE \quad \frac{i\left(E^2 - \frac{V^2}{4}\right) e^{2i\left(\frac{\left(E-\frac{V}{2}\right)}{\hbar v_F}x - \frac{\left(E+\frac{V}{2}\right)}{\hbar v_F}x'\right)}}{\hbar^3 v_F^3 \left(E(x-x') + \frac{V}{2}(x+x')\right)} \tag{A.190}$$

$$\chi = \left[\frac{ie^{-2iV(x+x')}\left(e^{i((2E(x-x')+V(x+x'))))}\left(1 - 2iE(x-x') + iV(x+x')\right)\right)}{8\hbar^3 v_F^3 (x-x')^3} \right. \\ \left. + \frac{ie^{-2iV(x+x')}\left(4V^2 x x' \mathrm{Ei}\left(i(2E(x-x') + V(x+x'))\right)\right)}{8\hbar^3 v_F^3 (x-x')^3} \right]_{-\infty}^{-\frac{V}{2}} \tag{A.191}$$