CONDUCTANCE IN A MESOSCOPIC SYSTEM BY METHOD OF NON-EQUILIBIRIUM GREEN'S FUNCTION

Research Internship Report

Submitted
by

KARTHIK S
Dept. of Physics
Central University of Karnataka

Under the Guidance of
Dr. Deepak Vaid

Dept. of Physics
National Institute of Technology - Karnataka
Surathkal,Mangalore - 575025
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DECLARATION

I hereby declare that the Research Internship report July 2017 entitled **CONDUCTANCE IN A MESOSCOPIC SYSTEM BY METHOD OF NON-EQUILIBIRIUM GREEN'S FUNCTION** which is being submitted to the National Institute of Technology, Karnataka, Surathkal, Department of Physics, is a bonafied report of the work carried out by me. The material contained in this report has not been submitted to any Universities or Institution for the award of any degree.

KARTHIK S
Department of Physics
Central University of Karnataka

PLACE : NIT-K,Surathkal

DATE : 10-07-2017

CERTIFICATE

This is to certify that the Research Internship report July 2017 entitled **CONDUCTANCE IN A MESOSCOPIC SYSTEM BY METHOD OF NON-EQUILIBIRIUM GREEN'S FUNCTION** submitted by Mr. KARTHIK S Dept. of Physics Central University of Karnataka(CUK) as the record of work carried out by him, is accepted as the Research Internship work report submission in Department of Physics. National Institute of Technology, Karnataka, Surathkal.

Dr. Deepak Vaid
Research Guide

Signature with Date and Seal

Dr. M. N. Satyanarayan
Head of the Department of Physics

Signature with Date and Seal

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ABSTRACT

In this project we intend to analyse the Non-Equilibirum Green's Function method of solving the tranport properties of a mesoscopic system. We derive the formula for conductance using the NEGF method (Landauer formalism). We also intend to analytically solve the conductance formula for a 1-D lattice connected to a source and a drain through a single channel. We simulate the same in the Kwant package and deeply analyse the results. We finally generate a generic code in the Kwant to calculate the conductance in a 1-D lattice with a real world environment. The analytical results are matched to the experimental results run in Kwant.

Contents

Chapter 1

INTRODUCTION

By the conventional Physics we know that the conductance of a conuducter is given by

$$S = \sigma \frac{A}{l}$$

where **S** is the conductance σ is the conductivity **A** being the area of cross-section and **l** being the length of the conductor

This above expression is applicable only in the ohmic regime. So we need to clearly understand what exactly is the ohmic regime. Now if the dimensions of the conductor is very large compared to (a)The mean-free path of the electrons in the conductor (b) The debroglie wavelength of the electrons in the conductor (c) The Phase-relaxation time, then the conductor is called ohmic conductor and will follow the ohmic laws. But when the dimensions of the conductor are comparable to the above mentioned length scales we find strange properties that do not anymore obey the ohm's law. We in this project handle such unique conductors and such a system which deals with these conductors are often called the mesoscopic systems(length scales involving a few nm to a few 1000nm)

The aim of this project is to understand the electrical properties of a conductor which is in the mesoscopic scale. In a very broad sense we are going to analyse the effects when a conductor of about 1/10th thick of a human hair is connected between the terminals of a battery (battery is a device which has two different chemical potential).The aim of this paper is to approach this problem in the Quantum mechanical way involving the laws of Quantum mechanics.Further more this Quantum mechanical treatment is known as the Landuaer approach and was initially carried out in the late 1960s to calculate the I-V characteristics of diodes and transistors. In the whole paper we would be following a few assumptions. Firstly we assume the 'Zero temperature' so that there is only one Energy 'E' in which the current can flow between the two chemical potentials. This means that we have only one one channel for conduction. In reality there is a band of energies that are allowed inside a solid.

We intend to calculate the conductance through this mesoscopic sample. We first calculate the Ballistic case (without scattering) and then the Scattering Case. We also analytically solve the conductance for a 1-D wire and also perform the same using the ***Kwant*** package. In this process we try to understand about the Greens function and how it leads in calculation of the system. First, Let us try to understand what exactly went wrong in the semiclassical way of doing such analysis.

1.1 The ideas of the Semi-Classical picture and its drawbacks

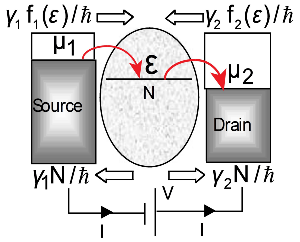
Initially in the 1960's the contacts made between the sample and the sources(usually current or the voltage) were ignored. This is because of the large size of the sample, hence the contact resistances made very little contribution to the over all conduction which can be ignored. As the technology was enhanced and the size of these sample/devices started to shrink the contact resistances were profound and the theory now demanded to include the contact resistances. In the semi-classical picture it was next to impossible to calculate the contact resistances. This is when the Quantum mechanical treatment was applied and one such successful method is the NEGF(Non-Equilibirium Greens Function) method.

Secondly there was no room for the broadening in the Energy of the channel in which it can conduct. The Semi-classical theory do not allow mismatched energy level between the contacts and the sample but in reality electrons with sligtly lower or higher energy did leak through the channel from the contacts. This could naturally be derived in the quantum mechanical treatment of the same problem.

Lastly , the very intersting part is that in the Semi-classical picture electrons are considered to be point-particles and therefore it cannot interfere like waves whereas the quantum treatments allows the electrons to behave like that of waves and this leads to successful explanation of the experimental results of the conductance in the channel with scattering(This is explained in detail in the chapter **10**).

1.2 Description of the System

The aim of the following few chapters is to calculate the expression for Ballistic conductance of a sample placed between two contacts using the NEGF. This paper also lets us calculate other parameters like the correlation function and charge density matrix using the NEGF



As in the figure 1.2 there is a sample **m** placed in between the two terminals i.e contact **1** and contact **2**. Now we have the sample that acts as a channel between the source and the drain.The channel does not have any scattering in it. Hence we have only the ballistic conductance that is responsible for the current. The two contacts here are approximated to be a electron rich and deficient Reservoirs. These electron densities in the reservoirs are hence given by the Fermi function.

The Fermi level of the contact **1** is relatively higher than the fermi level of the contact **2**.hence the chemical potentials (γ) are also of the form $\gamma_1 > \gamma_2$.
Now when the contacts and the sample are non-interacting then there is no flow of electrons between the contacts via the sample, but when the sample gets coupled/ starts interacting with the contacts there is a flow of electrons from contact **1** to the contact **2**.the Figure also shows the fermi level of the source and the drain

Now we have a system that comprises of three subsystem:

1. the contact **1** i.e the source.
2. the sample or the device .
3. the contact **2** i.e the drain.

Hence to know its conductance and other parameters one has to solve the hamiltonian of the whole system. The wavefunction describing the whole system is given by Ψ.
The wavefunction describing the contact **1** alone is given by ψ_1
The wavefunction describing the sample **m** alone is given by $\psi_{\mathbf{m}}$
The wave function describing the contact **2** is given by ψ_2

In the same manner

The coupling strength between the contact **1** and the sample is given by τ_1
The coupling strength between the contact **2** and the sample is given by τ_2

The coupling strength is measure of how well the sample is interacting with the contacts and is directly proportional to the relative time taken for electrons to pass from the contacts to the sample.

Therefore by applying all these information into the hamiltonian we get the following.

$$\begin{pmatrix} H_1 & \tau_1 & 0 \\ \tau_1^{\dagger} & H_{\mathbf{m}} & \tau_2 \\ 0 & \tau_2^{\dagger} & H_2 \end{pmatrix} \begin{pmatrix} |\psi_1\rangle \\ |\psi_{\mathbf{m}}\rangle \\ |\psi_2\rangle \end{pmatrix} = E \begin{pmatrix} |\psi_1\rangle \\ |\psi_{\mathbf{m}}\rangle \\ |\psi_2\rangle \end{pmatrix} \tag{1.1}$$

If we were to solve them then the first row multiplication would yield

$$H_1|\psi_1\rangle + \tau_1|\psi_{\mathbf{m}}\rangle = E|\psi_1\rangle$$

$$(E - H_1)|\psi_1\rangle = -\tau_1|\psi_{\mathbf{m}}\rangle \tag{1.2}$$

The above Equation resembles the perturbed hamiltonian equation given by

$$(E - H)|\psi\rangle = |\eta\rangle \tag{1.3}$$

where $|\eta\rangle$ is the perturbation.

Hence we are to solve this perturbed equation and this perturbation comes naturally through these equations.

In this paper we are to calculate the expression for the current through the channel. To calculate any of the transport parameter we should solve the above perturbed equation.When we solve the perturbed equation we will get two possible sets of **Wavefunctions**. We shall look into that deeper in the coming sections.

We try to express all of the parameters in terms of a peculiar function(Greens function) and hence by just knowing the Greens function it will be easy to calculate the parameters.

Chapter 2

GREEN'S FUNCTION

Green's function is a mathematical tool that lets us calculate a variety of time dependent expectation values.A green's function is defined as follows.

consider a operator Ô acting on a function $\phi(x)$ to give another function $\lambda(x)$

$$\hat{\mathbf{O}}\phi(x) = \lambda(x) \tag{2.1}$$

Then the Greens function for the operator $\hat{\mathbf{O}}$ at a point s is defined as

$$\hat{\mathbf{O}}G(x) = \delta(x - s) \tag{2.2}$$

In general case a Green's function is a 2 space-time coordinate. In this section we however deal with Non Equilibirum greens function since we have 3 sub-systems interacting with one another. The major difference between the Equilibirum Greens function and the Non-Equilibirium Greens function is that we have a few extra terms/factors relating to the interaction between the systems in the Non-equilibirum case

2.1 Non Equilibirum Greens Function

As discussed above we here make use of the Non Equilibirum Greens function and we are to find the NEFG of the Hamiltonian Operation hence the NEFG for the hamiltonian operator is thus

$$(E - H_i)G_i(E) = I \tag{2.3}$$

to solve the above equation we have from the equation 1.1

$$\begin{pmatrix} E - H_1 & \tau_1 & 0 \\ \tau_1^\dagger & E - H_\mathbf{m} & \tau_2 \\ 0 & \tau_2^\dagger & E - H_2 \end{pmatrix} \begin{pmatrix} G_1 & g_{1m} & g_{12} \\ g_{m1} & G_m & g_{2m} \\ g_{21} & g_{2m} & G_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{2.4}$$

In the above equation the capital G's corresponds to the Greens Funtion of the subsystem alone. where as the small g's are the Greens function corresponding to the combined system. In case of equilibiium the Greens function corresponding to the combined system will be zero, Hence reducing to the Equilibirium case.

$$\begin{pmatrix} E - H_1 & 0 & 0 \\ 0 & E - H_\mathbf{m} & 0 \\ 0 & 0 & E - H_2 \end{pmatrix} \begin{pmatrix} G_1 & 0 & 0 \\ 0 & G_m & 0 \\ 0 & 0 & G_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

There is no interaction between the subsystems hence the corresponding greens function vanishes and this is the Equilibirum Greens function for the non interacting system however we are interested in the interacting system

Non Equillibrium Greens Function(NEFG) are used in calculation of probablity current, conduction current.One can also calculate the total energy electron addition or removal energy using the method of NEGF . NEFG can be employed to extendend, as well as finite systems. By appropriate approximations in NEFG one can deduce the macroscopic laws.

Chapter 3

SELF ENERGIES

Self energy is the energy that the electron has as a result of changes that it itself causes in its environment. For example when the electron moves in the nano system it polarises the surrounding and hence in turn it develops a potential and hence a potential energy and is taken as the systems self energy. By solving the equation for the 1st row and the second column we could find out that

$$(E - H)g_{1m} + \tau_1 G_m = 0 \tag{3.1}$$

$$\tau_1^{\dagger} g_{1m} + (E - H_{\mathbf{m}})G_m + \tau_2 g_{2m} = I \tag{3.2}$$

$$\tau_2^{\dagger} G_m + (E - H_2)g_{2m} = 0 \tag{3.3}$$

from the equation 3.1 and 3.3

$$(E - H)g_{1m} = -\tau_1 G_m$$

$$\tau_2^{\dagger} G_m = -(E - H_2)g_{2m}$$

from the equation 2.3 we have

$$g_{1m} = -G_1^{'} \tau_1 G_m \tag{3.4}$$

similarly from the equation 3.3 we have

$$g_{2m} = -G_2^{'} \tau_2^{\dagger} G_m \tag{3.5}$$

Where the $G_1^{'}$ and $g_2^{'}$ are the Greens Function corresponding to the isolated contacts. Substituting the above equations 3.4 and 3.5 equation 3.2 we get the following result.

$$\tau_1^{\dagger} g_{1m} + (E - H_{\mathbf{m}})G_m + \tau_2 g_{2m} = I$$

$$-\tau_1^{\dagger} G_1^{'} \tau_1 G_m + (E - H_{\mathbf{m}})G_m - \tau_2 G_2^{'} \tau_2^{\dagger} G_m = I$$

$$(-\tau_1^{\dagger} G_1^{'} \tau_1 + (E - H_{\mathbf{m}}) - \tau_2 G_2^{'} \tau_2^{\dagger})G_m = I$$

$$G_m = (-\tau_1^{\dagger} G_1^{'} \tau_1 + (E - H_{\mathbf{m}}) - \tau_2 G_2^{'} \tau_2^{\dagger})^{-1} I$$

put $\tau_1^{\dagger} G_1 \tau_1 = \Sigma_1$ and $\tau_2 G_2 \tau_2^{\dagger} = \Sigma_2$

$$G_m = ((E - H_{\mathbf{m}}) - \Sigma_1 + -\Sigma_2)^{-1} I \tag{3.6}$$

From the above equation it is evident that the G_m is

$$G_m = ((E - H_{\mathbf{m}}) - \Sigma_1 - \Sigma_2)^{-1} \tag{3.7}$$

The Σ_1 and the Σ_2 are defined as the self energies corresponding to the source and drain of the system. Here the Self energy emerges out of the fact that contacts interact with the system and in turn changes the potential of the system. Usually the Contacts are made of metals which has a periodic nature and hence the G_1 and the $G2$ are calculated from the periodicity of these contacts

3.1 The Broadening matrix

As per the figure 1.2 the Electrons will flow from the Source via the sample. This can happen only when Electrons in the source has exactly the same energy to that of the channel. But by quantum mechanical arguments the energy may not exactly match with the channel energy still we might expect flow of electrons from the channel. the wavefuntion ψ at the interface of the source and the channel is given by

$$\psi = \frac{\sigma}{E - \epsilon + i\eta} \tag{3.8}$$

where the σ is the inflow rate term and in the denominator η is a small number. The above expression tells that the probability of transmission of a electron of energy **E** and a little away from the respective energy ϵ of the channel is non-zero. hence, we define the term Γ which is of the form

$$\Gamma \equiv i(\Sigma - \Sigma^{\dagger}) \tag{3.9}$$

The above expression is the expression for broadening and it arising purely due to quantum mechanical arguments. for a multi channel device the expression turns out to be a matrix and is called the broadening matrix.

3.2 The Spectral Function

The spectral function gives the measure to total number of states available in a particular system. Hence one can know the Density of states of the system by evaluating the spectral function in its appropriate limits.The spectral function in broad sense is the matrix version of the Density of States The spectral function is defined in the following fashion

$$A = 2\pi\delta(E - H) \tag{3.10}$$

The equation gives us the total number of states availabe for the system if we were to interpret this in terms of the wavefunctions that corresponds to the three subsystem them

$$A(\mathbf{r}, r', E) = 2\pi \sum_k \psi_k(\mathbf{r})\delta(E - \epsilon_k)\psi_k^*(r') \tag{3.11}$$

where k is a index that runs in the given subsystem.We can calculate the number of states occupied in that subsystem namely either the source the drain or the sample. We term this as the Local Density of states. To calculate the overall density of states we have to integrate allover the space that is simple add the Local Desity of States of all the subsystems. The total Density of States is given by

$$D(E) = \frac{1}{2}Tr(A(E)) = \sum_k \delta(E - \epsilon_k) \tag{3.12}$$

The above expression can also be expressed in terms of the Greens function hence by knowing the Greens function it lets us calculate the Density of States too. Equation 3.10 can be expressed as

$$2\pi\delta(E-\epsilon_k) = \frac{2\zeta}{(E-\epsilon_k)^2) + \zeta^2} \tag{3.13}$$

where ζ is a small number. now decoupling the above equation into the 2 parts we have

$$\frac{2\zeta}{(E-\epsilon_k)^2) + \zeta^2} = i\frac{1}{E-\epsilon_k + i\zeta} - i\frac{1}{E-\epsilon_k - i\zeta} \tag{3.14}$$

The first part of the equation can be named as the Retarded Greens function and the second part is the Advanced Greens function. We therefore denote the equation 3.10 as

$$A(E) = 2\pi(G - G^{\dagger}) \tag{3.15}$$

This section can be easily summarised as follows. When a electron tries to get into the sample there is a probabilty of it passing through the channel or it might be reflected from the channel hence there will be 2 wavefunction corresponding to this phenomena. 1. The refelected one and 2. the transmitted one and hence there are 2 sets of allowed values of energy for the eigen value equation. One for the reflected wavefunction and the other one for the transmitted wavefuntion hence there exist 2 Greens function corresponding to those energy and from the definition of equation 3.14 we find that the advance greens function is the complex conjugate of the retarded one.

We can also think of the spectral function as the following.
We define the Non-Equilibirum Greens function in the follwing way

$$G^n = G^R \sum_i \Gamma_i f(k, \gamma_i) G^A \tag{3.16}$$

Where the G^n is the no.of electrons in the given level. suppose if the levels is fully filled that it all the Fermi function $f(k, \gamma_i)$ is equal to 1 then it means that all the states are occupied hence the G^n gives the Density of the States. the G^R is the Retarded Greens function and is given by $G^R = (E - H + \sum_i \Gamma_i)$ and G^A is the Advance Greens Function $G^R = (E - H - \sum_i \Gamma_i)$hence

$$A = G^R \sum_i \Gamma_i G^A \tag{3.17}$$

3.3 Response to a incoming wave

From the previous section we find that we have 2 sets of wavefunction depending on what happens to the electron. The eigen value equation is of the form

$$(E - H)|\psi\rangle^R = |\psi\rangle^R$$

The above expression follows the arguements of the chapter **1** equation 1.3 hence the above expression can be rewritten as follows.

$$|\psi\rangle^R = G|\eta\rangle \tag{3.18}$$

similarly the equation of the advanced wavefunction can be written as

$$|\psi\rangle^A = G|\eta\rangle \tag{3.19}$$

Now let us analyse what happens when an electron which do not have enough energy to pass from the source to the drain comes at the interface of the source and the sample. The wavefunction corresponding to this electron has two parts one the reflected wavefunction and the other is the retarded response of the whole system to that wave. The wave function is of the form $|\psi_{1,n}\rangle + |\psi^R\rangle$ where the $|\psi_{1,n}\rangle$ is the wavefunction corresponding to the reflected electron when it is isolated and the wavefunction $|\psi^R\rangle$ corresponds to the response of the system when the source is connected. Now putting these in the Schrodinger equation we have

$$\begin{pmatrix} H_1 & \tau_1 & 0 \\ \tau_1^\dagger & H_{\mathbf{m}} & \tau_2 \\ 0 & \tau_2^\dagger & H_2 \end{pmatrix} (|\psi_{1,n}\rangle + |\psi^R\rangle) = E(|\psi_{1,n}\rangle + |\psi^R\rangle) \tag{3.20}$$

In the above equation the wavefunctions $\psi's$ are column matrices hence

$$|\psi_{1,n}\rangle = \begin{pmatrix} |\psi_{1,n}\rangle \\ 0 \\ 0 \end{pmatrix} \tag{3.21}$$

similarly

$$|\psi^R\rangle = \begin{pmatrix} |\psi_1^R\rangle \\ |\psi_m^R\rangle \\ |\psi_2^R\rangle \end{pmatrix} \tag{3.22}$$

Putting back the above equations in to the hamiltonian we get the following :

$$\begin{pmatrix} H_1 & \tau_1 & 0 \\ \tau_1^\dagger & H_{\mathbf{m}} & \tau_2 \\ 0 & \tau_2^\dagger & H_2 \end{pmatrix} \begin{pmatrix} |\psi_{1,n}\rangle \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} H_1 & \tau_1 & 0 \\ \tau_1^\dagger & H_{\mathbf{m}} & \tau_2 \\ 0 & \tau_2^\dagger & H_2 \end{pmatrix} \begin{pmatrix} |\psi_1^R\rangle \\ |\psi_m^R\rangle \\ |\psi_2^R\rangle \end{pmatrix} = E \begin{pmatrix} |\psi_{1,n}\rangle \\ 0 \\ 0 \end{pmatrix} + E \begin{pmatrix} |\psi_1^R\rangle \\ |\psi_m^R\rangle \\ |\psi_2^R\rangle \end{pmatrix}$$

Now on rearranging the terms we have

$$\begin{pmatrix} H_1|\psi_{1,n}\rangle \\ \tau_1^\dagger|\psi_{1,n}\rangle \\ 0 \end{pmatrix} + \begin{pmatrix} H_1 & \tau_1 & 0 \\ \tau_1^\dagger & H_{\mathbf{m}} & \tau_2 \\ 0 & \tau_2^\dagger & H_2 \end{pmatrix} \begin{pmatrix} |\psi_1^R\rangle \\ |\psi_m^R\rangle \\ |\psi_2^R\rangle \end{pmatrix} = E \begin{pmatrix} |\psi_{1,n}\rangle \\ 0 \\ 0 \end{pmatrix} + E \begin{pmatrix} |\psi_1^R\rangle \\ |\psi_m^R\rangle \\ |\psi_2^R\rangle \end{pmatrix}$$

Further more we have

$$\begin{pmatrix} E|\psi_{1,n}\rangle - E|\psi_{1,n}\rangle \\ \tau_1^\dagger|\psi_{1,n}\rangle \\ 0 \end{pmatrix} = \begin{pmatrix} E - H_1 & \tau_1 & 0 \\ \tau_1^\dagger & E - H_{\mathbf{m}} & \tau_2 \\ 0 & \tau_2^\dagger & E - H_2 \end{pmatrix} \begin{pmatrix} |\psi_1^R\rangle \\ |\psi_m^R\rangle \\ |\psi_2^R\rangle \end{pmatrix}$$

$$\begin{pmatrix} 0 \\ \tau_1^\dagger|\psi_{1,n}\rangle \\ 0 \end{pmatrix} = \begin{pmatrix} E - H_1 & \tau_1 & 0 \\ \tau_1^\dagger & E - H_{\mathbf{m}} & \tau_2 \\ 0 & \tau_2^\dagger & E - H_2 \end{pmatrix} \begin{pmatrix} |\psi_1^R\rangle \\ |\psi_m^R\rangle \\ |\psi_2^R\rangle \end{pmatrix}$$

$$\begin{pmatrix} |\psi_1^R\rangle \\ |\psi_m^R\rangle \\ |\psi_2^R\rangle \end{pmatrix} = G \begin{pmatrix} 0 \\ \tau_1^\dagger|\psi_{1,n}\rangle \\ 0 \end{pmatrix} \tag{3.23}$$

from the equation 2.4 we get

$$\begin{pmatrix} |\psi_1^R\rangle \\ |\psi_m^R\rangle \\ |\psi_2^R\rangle \end{pmatrix} = \begin{pmatrix} G_1 & g_{1m} & g_{12} \\ g_{m1} & G_m & g_{2m} \\ g_{21} & g_{2m} & G_2 \end{pmatrix} \begin{pmatrix} 0 \\ \tau_1^\dagger|\psi_{1,n}\rangle \\ 0 \end{pmatrix} \tag{3.24}$$

We can now know the wavefunctions too from the Green's function.

$$|\psi_m^R\rangle = G_m\tau_1^\dagger|\psi_{1,n}\rangle \tag{3.25}$$

in the same manner

$$|\psi_2^R\rangle = g_{2m}\tau_1^\dagger|\psi_{1,n}\rangle$$

We know from equation 3.5 the value of g_{2m} is substituted and hence we can end up getting the following expression

$$|\psi_2^R\rangle = G_2\tau_2^\dagger G_m\tau_1^\dagger|\psi_{1,n}\rangle \tag{3.26}$$

here the $|\psi_m^R\rangle = \psi_m$ since there is no other wavefunction other than the samples. In the same manner $|\psi_2^R\rangle = |\psi_2\rangle$ But in the source we have the reflected and the response wavefunction , Hence the total wavefunction $|\psi_1\rangle = |\psi_{1,n}\rangle + |\psi_1^R\rangle$ Therefore

$$|\psi_1\rangle = |\psi_{1,n}\rangle + G_1\tau_1 G_m\tau_1^\dagger|\psi_{1,n}\rangle$$

$$|\psi_1\rangle = (1 + G_1\tau_1 G_m\tau_1^\dagger)|\psi_{1,n}\rangle \tag{3.27}$$

Hence by just knowing the wavefunction that comes in we can deduce all the solutions to the wavefunctions of the subsystems.

Chapter 4

THE PROBABILTY CURRENT

The rate of change of the probability density is called as the probability current and we can evaluate this by just differentiating the probability density with time.We are here to calculate the probability at steady state

$$\frac{\partial}{\partial t}|\psi_i|^2 = 0 = \sum_i \frac{\partial \langle\psi|i\rangle\langle i|\psi\rangle}{\partial t} \tag{4.1}$$

Simplification of the expression yields

$$\sum_i \left(\frac{\partial \langle\psi|i\rangle}{\partial t}\langle i|\psi\rangle + \langle\psi|i\rangle\frac{\partial \langle i|\psi\rangle}{\partial t} \right)$$

From schrodinger Time dependent equation we have

$$-i\hbar\frac{\partial \Phi}{\partial t} = H\Phi \tag{4.2}$$

Therefore the expression reduces to

$$\frac{i}{\hbar}\sum_i (\langle\psi|H|i\rangle\langle i|\psi\rangle - \langle\psi|i\rangle\langle i|H|\psi\rangle) = 0 \tag{4.3}$$

Here the wavefunction ψ represents the wavefunction of the whole system. now **i** runs only in the subspace of the sample hence this equation is basically projection of the entire wavefunction on to the device subspace and hence it yields the following

$$\frac{i}{\hbar}\sum_i (\langle\psi|H|\psi_m\rangle - \langle\psi_m|H|\psi\rangle) = 0 \tag{4.4}$$

Here we have

$$\langle\psi| = \begin{pmatrix} \psi_1^* & \psi_m^* & \psi_2^* \end{pmatrix}$$

$$H = \begin{pmatrix} H_1 & \tau_1 & 0 \\ \tau_1^\dagger & H_{\mathbf{m}} & \tau_2 \\ 0 & \tau_2^\dagger & H_2 \end{pmatrix}$$

$$|\psi_m\rangle = \begin{pmatrix} 0 \\ \psi_m \\ 0 \end{pmatrix}$$

in the same manner

$$|\psi\rangle = \begin{pmatrix} |\psi_1\rangle \\ |\psi_m\rangle \\ |\psi_2\rangle \end{pmatrix}$$

$$\langle\psi_m| = \begin{pmatrix} 0 & \psi_m^* & 0 \end{pmatrix}$$

Now putting these values in the equation 4.4 we have the following
The expression of $\langle\psi|H|\psi_m\rangle$ is

$$\begin{pmatrix} \psi_1^* & \psi_m^* & \psi_2^* \end{pmatrix} \begin{pmatrix} H_1 & \tau_1 & 0 \\ \tau_1^\dagger & H_{\mathbf{m}} & \tau_2 \\ 0 & \tau_2^\dagger & H_2 \end{pmatrix} \begin{pmatrix} 0 \\ \psi_m \\ 0 \end{pmatrix} = \psi_1^*\tau_1\psi_m + \psi_m^* H_m \psi_m + \psi_2^*\tau_2^\dagger\psi_m$$

similarly the expression for $\langle\psi_m|H|\psi\rangle$ is

$$\begin{pmatrix} 0 & \psi_m^* & 0 \end{pmatrix} \begin{pmatrix} H_1 & \tau_1 & 0 \\ \tau_1^\dagger & H_{\mathbf{m}} & \tau_2 \\ 0 & \tau_2^\dagger & H_2 \end{pmatrix} \begin{pmatrix} |\psi_1\rangle \\ |\psi_m\rangle \\ |\psi_2\rangle \end{pmatrix} = \psi_m^*\tau_1^\dagger\psi_1 + \psi_m^* H_m \psi_m + \psi_m^*\tau_2\psi_2$$

Hence substituting the values of $\langle\psi|H|\psi_m\rangle$ and $\langle\psi_m|H|\psi\rangle$ in the equation 4.4 and rearranging

$$\frac{i}{\hbar}([\langle\psi_1|\tau_1|\psi_m\rangle - \langle\psi_m|\tau_1^\dagger|\psi_1\rangle] + [\langle\psi_2|\tau_2|\psi_m\rangle - \langle\psi_m|\tau_2^\dagger|\psi_2\rangle]) = 0 \tag{4.5}$$

If not in the steady state and to calculate the current we multiply the equation by the charge. hence the Probability current ($\mathbf{j}$) is given by

$$j_i = \frac{ie}{\hbar}(\langle\psi_i|\tau_i|\psi_m\rangle - \langle\psi_m|\tau_i^\dagger|\psi_i\rangle) \tag{4.6}$$

In the steady state the first term in the equation 4.5 is defined as the incoming probability current into the device from the source and the second is the probability current due to the drain.
In the non equilibirum case these lead to a non-zero current and that can be caluclated by the equation above.

Chapter 5

THE ELECTRICAL CURRENT IN THE CHANNEL

Using the equation in the previous section we can calculate the electrical current through the channel to the drain hence the drain current is calculated as follows

Before calculating the current let us define the broadening matrix in a slightly different manner. The broadening matrix Γ can be expressed in terms of the spectral function as follows

$$\Gamma_i = \tau_i^\dagger A_i \tau_i = i(\Sigma_i - \Sigma_i^\dagger) \tag{5.1}$$

Now we calculate the drain current j_2 the drain current due to the incoming wave of energy 'E' is given by

$$j_2 = \frac{ie}{\hbar}(\langle\psi_2|\tau_2|\psi_m\rangle - \langle\psi_m|\tau_2^\dagger|\psi_2\rangle) \tag{5.2}$$

ψ_2 and ψ_m can be expressed in terms of the reflected wavefunction $\psi_{1,n}$ putting the value of the wavefunction in the above equation we have

$$j_2 = \frac{ie}{\hbar}(\langle\psi_{1,n}|G_2'^\dagger \tau_2 G_m^\dagger \tau_1 G_m \tau_1^\dagger|\psi_{1,n}\rangle - \langle\psi_{1,n}|G_m^\dagger \tau_1 G_2' \tau_2^\dagger G_m \tau_1^\dagger|\psi_{1,n}\rangle) \tag{5.3}$$

Simplifying the equation we have.

$$j_2 = \frac{ie}{\hbar}(\langle\psi_{1,n}|\tau_1 G_m^\dagger \tau_2^\dagger (G'^\dagger - G')\tau_2 G_m \tau_1^\dagger|\psi_{1,n}\rangle) \tag{5.4}$$

As per the definition in the equation 5.1

$$j_2 = \frac{e}{\hbar}\langle\psi_{1,n}|\tau_1 G_m^\dagger \Gamma_2 G_m \tau_1^\dagger|\psi_{1,n}\rangle \tag{5.5}$$

To calculate the overall current we have to integrate over all the possible energies. hence

$$j_2 = \frac{2e}{\hbar}\int_{E=-\infty}^{\infty} dE f(E,\gamma_1)\sum_n \delta(E - E_n)\langle\psi_{1,n}|\tau_1 G_m^\dagger \Gamma_2 G_m \tau_1^\dagger|\psi_{1,n}\rangle \tag{5.6}$$

where the factor **2** comes due to the spin and the function $f(E,\gamma_1)$ is the fermi function of the source. further simplification will yield

$$j_2 = \frac{2e}{\hbar}\int_{E=-\infty}^{\infty} dE f(E,\gamma_1)\sum_{n,k} \delta(E - E_n)\langle\psi_{1,n}|\tau_1|k\rangle\langle k|G_m^\dagger \Gamma_2 G_m \tau_1^\dagger|\psi_{1,n}\rangle \tag{5.7}$$

Where we apply the identity operator in the above expression now, Rearranging the terms and even more simplifying we get

$$j_2 = \frac{2e}{\hbar}\int_{E=-\infty}^{\infty} dEf(E,\gamma_1)\sum_k \langle k|G_m^\dagger \Gamma_2 G_m \tau_1^\dagger \frac{A_1}{2\pi}\tau_1|k\rangle \tag{5.8}$$

$$j_2 = \frac{2e}{\hbar}\int_{E=-\infty}^{\infty} dEf(E,\gamma_1)Tr(G_m^\dagger \Gamma_2 G_m \Gamma_1) \tag{5.9}$$

Here we have assumed that the fermi function of the drain is **0** but generally it is not zero hence we have to subract the fermi function of that too

The total current **J** is given by

$$j_2 = \frac{2e}{\hbar}\int_{E=-\infty}^{\infty} dE(f(E,\mu_1)-f(E,\mu_2))Tr(G_m^\dagger \Gamma_2 G_m \Gamma_1) \tag{5.10}$$

This is the **Landauer** formula for the current.

Chapter 6

Correlation function and a different approach to the problem

6.1 GREEN'S FUNCTION A DIFFERENT APPROACH

We here try to analyse a few things in a conceptual way. Let us assume that scenario in the figure 1.the Source is connected to the sample and inturn sample connected to the drain. Now the electron distributions in the reserviors are given by the Fermi function. The difference in the fermi energy drives the system out of equilibirium and thereby causing a current to flow through the system. We here write the total hamiltonian of the system to be

$$[E]\psi = [H]\psi + [\Sigma]\{\psi\} + \{s\} \tag{6.1}$$

where the term Σ is the connection to the contacts i.e it tells about the extraction of the electrons from the contacts and the term s is the source term. It tells about the sources invoved in the system i.e injection of the electrons from the sources.For one electron one channel problem the paramters are just numbers but generally the parameters are of the form of a matrix. Now rearranging the terms we have

$$([E] - [H] - [\Sigma_1] - [\Sigma_2])\{\psi\} = \{s\} \tag{6.2}$$

Hence

$$\{\psi\} = \frac{\{s\}}{([E] - [H] - [\Sigma_1] - [\Sigma_2])} \tag{6.3}$$

Where we define the greens function to be

$$G = ([E] - [H] - [\Sigma_1] - [\Sigma_2])^{-1} \tag{6.4}$$

We calculate the probability of a electron slightly higher or lower than the energy required to enter the level , then it turns out to be non-Zero. This means that there exist a broadening in the spectrum where mismatched energy levels too can escape through the channel and we define this broadening matrix to be

$$\Gamma_i \equiv i(\Sigma_i - \Sigma_i^{\dagger}) \tag{6.5}$$

Where Γ_i is the Broadening matrix discussed in the chapter 2 section 3.1.

6.2 CORRELATION FUNCTION AND RELATION TO THE SPECTRAL FUNCTION

By the second quantisation we have the correlation function or sometimes called as non-equilibirum Green's function to be of the form

$$G^{m}_{i,j}(t,t^{'}) \equiv \langle c^{\dagger}_{j}(t^{'})c_{i}(t)\rangle \tag{6.6}$$

where $c^{\dagger}_{i}$ and c_i are the creation and annihilation operators for an electron at the **i**th state. In the steady state the above equation in terms of energy gives the energy density at a point. In equilibirium case the electron density is given by the fermi function in the reservoirs. Hence the correlation function and the spectral function is related as follows

$$G^{n}_{eq} = A(E)f(E-\gamma) \tag{6.7}$$

To understand the above equation we need to understand the terms, the term G^n. It is like the electronic density at a given energy. Its like the probability density of electrons in that level. Hence we calculate the $\psi\psi^{\dagger}$ to know the G^n

$$G^{n} = \{\psi\}\{\psi^{\dagger}\} = G\{s\}\{s^{\dagger}\}G^{\dagger} \tag{6.8}$$

We here define $\{s\}\{s^{\dagger}\} = \Sigma^{in}$ and it physically means the strength of the source hence we have

$$G^{n} = G\Sigma^{in}G^{\dagger} \tag{6.9}$$

this is termed as the non-equilibirum correlation function .Here we can also further deduce the strength to be

$$\Sigma^{in} = \sum_{i} \Gamma_{i} f(E,\gamma_{i})$$

This leads to defining the Spectral function when $f(E,\gamma_i) = 1$ we have the the density of states and hence

$$A(E) = G\sum_{i} \Gamma_{i} G^{\dagger}$$

Chapter 7

FEW MORE USEFUL RESULTS AND SUMMARY SO FAR

We can also calculate the Charge density matrix in the same manner as we did for the current we have to calculate the charge density matrix for a given energy E and intergrate it over all the energies. the charge Density matrix is given by

$$\rho = \sum_{k} f(k, \gamma) |\psi_k\rangle\langle\psi_k| \tag{7.1}$$

and the function $f(k, \gamma)$ is the number density function. For a ideal source its given by its fermi function and following the steps we followed for calculating the current we have

$$\rho = \frac{1}{\pi} \int_{E=\infty}^{\infty} dE f(e, \gamma_i) G_m \Gamma_i G_m^{\dagger} \tag{7.2}$$

In the above sections we have analysed how to derive the Current through a single channel device. For a multi channel device the hamiltonian matrix of the system will consist of more elements there by increasing its dimensionalities. In the whole of this paper we have assumed that we nearest neighbouring toght bending model and hence we safely asssumed that the channels are not branched amongest one another.

Also the whole of this paper has assumed no scattering taking place in the sample but in real situations scattering do happen in the sample and we have to account for the scattering too and is accounted by another self energy term $\Sigma_{\mathbf{s}}$. There will be a scattering term also to account for in the hamiltonian. Also in a multi-channel device it acts as it has more than one source since there are N channels to conduct. nevertheless this example is a classic one to start with the quantum tranport phenomena

We also should note that these effects are observable only at low temperatures since the Fermi function of these reservoirs or the occupation number of electrons strongly depend on the temperature at higher temperature we do not see any quantum effects it will be classical however making appropriate approximations to the NEFG we can achieve the classical results.

Here is the methodology of working with majority of NEFG Problems in calculation of any of its transport parameters

1. Look for the types and no.of interactions in the system
2. Write down the Hamiltonian of the system
3. Calculate the self-energies and compute its matrix
4. Calculate the Greens function by the definition in the equation 3.7
5. Using the Green's function now we deduce the tranport parameter by suitable formula.

Chapter 8

SOLVING SOME EXAMPLES

Let us see how self energies are calculated thereby leading to deduce the Green's function. The aim of this section is to calculate the Self energies for a 1-D lattice that is regularly arranged with a lattice spacing **'a'**.

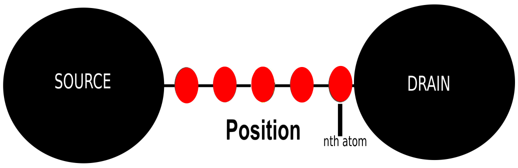
Recalling some of the useful formulas

$$\Sigma = \tau_i G' \tau_i^\dagger$$

$$\Gamma = i(\Sigma_i - \Sigma_i^\dagger)$$

$$G^R = [EI - H - \Sigma_1 - \Sigma_2]$$

$$\sigma(conductance) = \frac{2e^2}{\hbar} Tr(G_m^\dagger \Gamma_2 G_m \Gamma_1)$$



There is a 1-D lattice with spacing **'a'** and leads are connected to both the ends of the lattice. Our aim is to calculate the Self energies(Σ's) for this system. The advantage of using the NEFG is that we can bypass the accounting of the contacts between source and the sample. this interface interaction is inherently taken care by the self energies. All we have to do is to calculate the **H**'s and Σ''s in isolation.

If we calculate the Hamiltonian Equation for sample

$$E \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \dots \\ \Psi_n \end{pmatrix} = [H] \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \dots \\ \Psi_n \end{pmatrix} \tag{8.1}$$

$$[H] = \begin{pmatrix} \epsilon & \tau & 0 & \dots & & \\ \tau & \epsilon & \tau & 0 & \dots & \\ 0 & \tau & \epsilon & \tau & 0 & \dots \\ \dots\dots & & & & & \\ \dots\dots & & & & & \end{pmatrix} \tag{8.2}$$

Let us assume an electron is travelling from left to right. As in the figure the contacts are connected to the right of n'th atom. Writing the Expression for wavefunction corresponding to the nth atom

$$E\Psi_n = \tau\Psi_{n-1} + \epsilon\Psi_n + \tau\Psi_{n+1} \tag{8.3}$$

By applying the open Boundary condition

$$\Psi_n = \Psi_0 e^{ikna} \tag{8.4}$$

therefore the Ψ_{n+1} is given by

$$\Psi_{n+1} = \Psi_0 e^{ik(n+1)z}$$

$$\Psi_{n+1} = \Psi_n e^{ika} \tag{8.5}$$

$$E\Psi_n = \tau\Psi_{n-1} + (\epsilon + \tau e^{ikz})\Psi_n \tag{8.6}$$

Here Ψ_{n-1} may not always follow the argument in the equation 8.4 because the lattice may be different Now lets write down the hamiltonian of the sample

The right most part in the equation 8.6 is like the extra term added to the energy and hence τe^{ika} is the self energy term added. We therefore conclude that

$$\Sigma_2 = \begin{pmatrix} 0 & 0 & 0 & ... \\ 0 & 0 & 0 & ... \\ ... & & & \\ ... & & & \\ ...... & 0 & 0 & \tau e^{ikz} \end{pmatrix} \tag{8.7}$$

Following the same arguments and procedures we write

$$\Sigma_1 = \begin{pmatrix} \tau e^{ikz} & 0 & 0 & ... \\ 0 & 0 & 0 & ... \\ ... & & & \\ ... & & & \\ ...... & 0 & 0 & 0 \end{pmatrix} \tag{8.8}$$

The above equations are the self energies corresponding to any 1-D regular lattice. hence the corresponding Greens function is

$$G^{-1} = \begin{pmatrix} E - H - \tau e^{ikz} & \tau & 0 & ... & \\ \tau & E - H & \tau & .... & \\ .... & .... & .... & \tau & E - H - \tau e^{ikz} \end{pmatrix} \tag{8.9}$$

From here we can calculate the Γ's and other parameters needed for conductance.

Now let us calculate the allowed energies inside our lattice. Since our lattice is a 1-D lattice we write equation 8.3

$$E\Psi_n = \tau\Psi_{n-1} + \epsilon\Psi_n + \tau\Psi_{n+1}$$

Our lattice is periodic

$$\Psi_n = \Psi_0 e^{ikna}$$

$$\Psi_{n+1} = \Psi_n e^{ika}$$

$$\Psi_{n-1} = \Psi_0 e^{-ika}$$

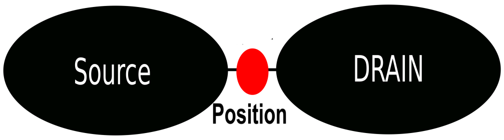
$$E\Psi_n = \tau\Psi_n e^{-ika} + \epsilon\Psi_n + \tau\Psi_n e^{ika}$$

$$E = \epsilon + 2\tau\cos(ka) \tag{8.10}$$

The energy values equal to the above expression can only be transmitted in the channel .

8.1 Conductance through 1-site 1-D lattice

Now let us calculate for a simple 1-site without any scattering.



here Greens function for the system is

$$G = [EI - H - \Sigma_1 - \Sigma_2]^{-1} \tag{8.11}$$

Since its just a 1-Site potential all the Parameters are a 1X1 Matrix

$$G = [EI - H - 2\tau e^{ika}]^{-1}$$

calculating the Γ's (Refer the formula in the beginning of this section)

$$\Gamma_1 = i(\tau e^{ika} - \tau e^{-ika})$$

$$\Gamma_1 = 2\tau\sin(ka)$$

simillarly

$$\Gamma_2 = 2\tau\sin(ka)$$

$$G = \frac{1}{E - \epsilon - 2\tau e^{ika}} \tag{8.12}$$

$$G^\dagger = \frac{1}{E - \epsilon - 2\tau e^{-ika}} \tag{8.13}$$

From the formula for conductance

$$\Gamma_1 G \Gamma_2 G^\dagger = 2\tau\sin(ka).\frac{1}{E - \epsilon - 2\tau e^{ika}}.2\tau\sin(ka).\frac{1}{E - \epsilon - 2\tau e^{ika}} \tag{8.14}$$

$$\Longrightarrow \frac{4\tau^2\sin^2(ka)}{(E-\epsilon)^2 - (E-\epsilon)(4\tau\cos(ka)) + 4\tau^2}$$

From the equation 8.10 putting value of $E - \epsilon$

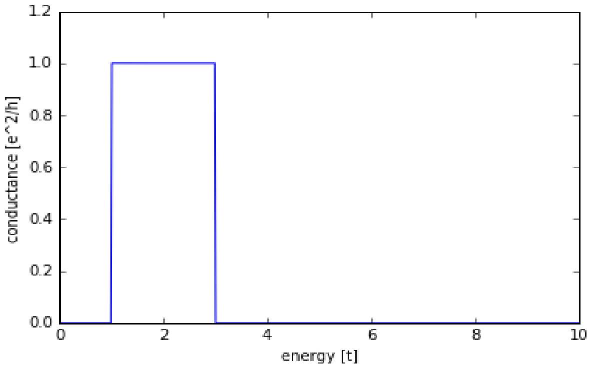
$$\frac{4\tau^2\sin^2(ka)}{4\tau^2\cos^2(ka) - 8\tau^2\sin^2(ka) + 4\tau^2}$$

$$\frac{4\tau^2\sin^2(ka)}{4\tau^2(1 - \cos^2(ka))} = 1 = T(E) \tag{8.15}$$

where T(E) is the transmission function hence the conductance is given to be

$$\sigma(conductance) = \frac{2e^2}{\hbar} \tag{8.16}$$

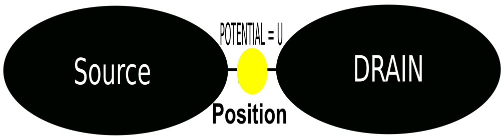
If we were to plot the conductance as a function of energy we get



electrons with Energy in between $E - \epsilon$ and $E + \epsilon$ will pass through the channel.

8.2 Conductance through 1-site 1-D lattice with scattering

See the figure below



This problem is very similar to the previous one except that there exist a potential U at the atomic site other than the onsite energy ϵ. hence the hamiltonian of the system will look like

$$H = \epsilon + \mathbf{U} \tag{8.17}$$

therefore the Green's function will look like

$$G = [E - \epsilon - \mathbf{U} - 2\tau e^{ika}]^{-1} \tag{8.18}$$

Decoupling the above equation into real and imaginary parts we have

$$G = \frac{1}{(E - \epsilon - 2\tau\cos(ka)\mathbf{U}) - i2\tau\sin(ka)}$$

Following the arguements of the previous section, From the equation 8.10 we write

$$G = \frac{1}{-\mathbf{U} - i2\tau\sin(ka)} \tag{8.19}$$

therefore we can calculate the $G^\dagger$ to be

$$G^\dagger = \frac{1}{-\mathbf{U} + i2\tau\sin(ka)} \tag{8.20}$$

$$\Gamma_1 = 2\tau\sin(ka) \tag{8.21}$$

$$\Gamma_2 = 2\tau \sin(ka) \tag{8.22}$$

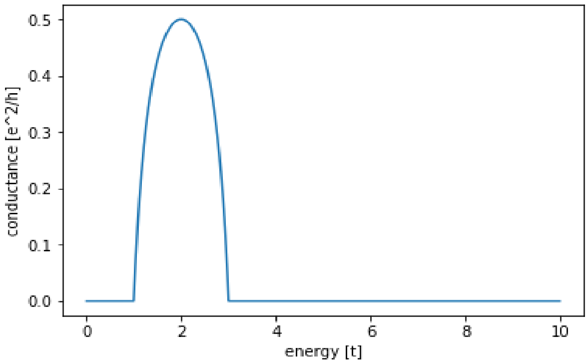
and now the value of conductance from the above equations will turn out to be

$$\sigma(conductance) = \frac{2e^2}{h}\Gamma_1 G \Gamma_2 G^\dagger = \frac{4\tau^2 \sin^2(ka)}{\mathbf{U} + 4\tau^2 \sin^2(ka)} \tag{8.23}$$

in terms of the energy **E** we get

$$\sigma(conductance) = \frac{4\tau^2 - (E-\epsilon)^2}{\mathbf{U}^2 + 4\tau^2 - (E-\epsilon)^2} \tag{8.24}$$

Now plotting the conductance as a function of energy we have



8.3 Conductance in a 1-D lattice with 2-sites

Now this problem is the exact same way of solving any sites. Lets us suppose we have **n** sites then the hamiltonian of that lattice is going to be a **nxn** matrix. Hence if we can solve for 2 lattice the same results will be applying for any no.of lattice points refer the figure 8 and instead of having n sites we have 2 sites. We then write down the hamiltonian of the system. The hamiltonian of a 2-site 1-D system is

$$H = \begin{pmatrix} \epsilon & \tau \\ \tau & \epsilon \end{pmatrix} \tag{8.25}$$

The self energies are given by

$$\Sigma_1 = \begin{pmatrix} \tau e^{ika} & 0 \\ 0 & 0 \end{pmatrix} \tag{8.26}$$

$$\Sigma_2 = \begin{pmatrix} 0 & 0 \\ 0 & taue^{ika} \end{pmatrix} \tag{8.27}$$

$$G = [E[I] - [H] - [\Sigma_1] - [\Sigma_2]]^{-1} \tag{8.28}$$

Solving the above equation using the condition 8.10 we have the Green's function of the system to be

$$G = \frac{1}{\tau^2(e^{-i2ka} - 1)} \begin{pmatrix} \tau e^{-ika} & \tau \\ \tau & \tau e^{-ika} \end{pmatrix} \tag{8.29}$$

The $G^\dagger$ will be

$$G^\dagger = \frac{1}{\tau^2(e^{i2ka} - 1)} \begin{pmatrix} \tau e^{ika} & \tau \\ \tau & \tau e^{ika} \end{pmatrix} \tag{8.30}$$

The broadening matrices Γ_1 and Γ_2 is given by

$$\Gamma_1 = \begin{pmatrix} 2\tau\sin(ka) & 0 \\ 0 & 0 \end{pmatrix} \tag{8.31}$$

$$\Gamma_2 = \begin{pmatrix} 0 & 0 \\ 0 & 2\tau\sin(ka) \end{pmatrix} \tag{8.32}$$

Hence the value of $Tr(\Gamma_1 G \Gamma_2 G^\dagger)$ is

$$Tr(\Gamma_1 G \Gamma_2 G^\dagger) = \frac{4\tau^4\sin^2(ka)}{\tau^4(e^{i2ka}-1)(e^{-i2ka}-1)} = 1 \tag{8.33}$$

This equation on further simplification will yield **1**.

$$\sigma(conductance) = \frac{2e^2}{h} \tag{8.34}$$

Hence if there are no scattering then the conductance through that channel is basically a constant in that energy range iot really doesnt matter if there is 1-site or **n**-site. the analytical results also here are the same and hence the same for the graphs

Its quite convincing because when we have a perfect interaction between the atoms the arrangement is just like a 1-D quantum barrier with barrier thickness going to 0 problem and if the electron has the right energy then it is sure of passing through the barrier.

8.4 Conductance in a 1-D lattice with 2-sites with one scatterer

In this section let us not solve numerically but try to put forward some arguments based on previous results. The arguments are quite simple. here the electron faces a issue the potential it feels at the site is different from the others hence there is a disturbance in the hence here is the a barrier with the thickness. now the energy close to $E-\epsilon$ and $E+\epsilon$ has less probabilty of crossing the barrier and as the energy is close to **E** there is maximum chance of tunnelling. in this way the results will exactly be the same as we seen in the section **8.2**.

Chapter 9

Kwant Simulations And Numerical Experiment

9.1 Working with the Kwant

Kwant is a free (open source) Python package for numerical calculations on tight-binding models with a strong focus on quantum transport. It is designed to be flexible and easy to use.
Tight-binding models can describe a vast variety of systems and phenomena in quantum physics. Therefore, Kwant can be used to simulate

1. Metals,
2. Graphene,
3. Topological insulators,
4. Quantum Hall effect,
5. Superconductivity,
6. Spintronics,
7. Molecular electronics,
8. Any combination of the above, and many other things.

Kwant can calculate

1. Transport properties (conductance, noise, scattering matrix).
2. Dispersion relations.
3. Wave functions.
4. Various Green's functions.
5. Out-of-equilibrium local quantities.
6. Modes.

Other computations involving tight-binding Hamiltonians can be implemented easily.

We use the Kwant package to simulate a 1-D lattice and calculate its conductance through that lattice. The general working in Kwant is as follows

1. Define the lattice you want to create. The kwant works assuming the tight bending approximations
2. Now set the On-site energies i.e the Energies at every lattice point and also specify the interaction between the lattice points usually the interaction is called the hoppings. Set how the electrons will hop between the neighbors
3. Attach your lattice to the source or the drain or both appropriately . There can be many source attached to different sites. In the context of Kwant it is termed as 'Attaching the leads to the system'
4. Now give different values of energy to the incoming electron and let the Kwant calculate the scattering matrix and the conductance for those energies.
5. Plot the result using an desired method it can be easily implemented by the use of matplotlib

9.2 The Tight Bending Approximation: A brief look

In the tight-binding model we assume the opposite limit to that used for the nearly-free-electron ap- proach, i.e. the potential is so large that the electrons spend most of their lives bound to ionic cores, only occasionally summoning the quantum-mechanical wherewithal to jump from atom to atom.
We also assume that the atoms in the atomic lattice interacts only with their nearest neighbouring atoms and the interaction with any other atom is essentially zero.

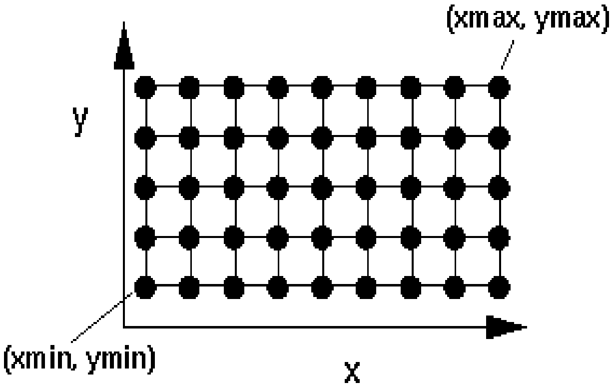
The electrons cannot stay anywhere in between two atoms therefore the hamiltonian of this lattice is no more a continuous one it is a discrete hamiltonian and discrete hamiltonian for a 2-D regular lattice is given by

$$H = \sum_{i,j} \left[\left(V(ai,aj) + 4\tau\right) |i,j\rangle\langle i,j| - \tau\big(|i+1,j\rangle\langle i,j| + |i,j\rangle\langle i+1,j| + |i,j+1\rangle\langle i,j| + |i,j\rangle\langle i,j+1|\big)\right] \tag{9.1}$$

where τ is defined as

$$\tau = \frac{\hbar^2}{2ma^2}$$

'm' is the effective mass of the incoming particle
'a' is the lattice parameter here is how the lattice will look



9.3 The Numerical Experiment

In this section we run a numerical experiment on calculating the conductance through a near 1-D lattice. We say Near because the Kwant packages do not have the option of calculating the conductance through a 1-D lattice.

As per the method if working in kwant we first create the lattice. we create a 2-D lattice with just 2 rows.

Next we plug in the On-Site potentials, here to make the system look 1-D we set all the potentials on the row 1 to be zero. In the same manner we also set the hopping term in the vertical direction to be zero.

In the process of attaching the leads we set attach the leads to the two ends of the lattice and make the interaction between the leads and the lattice in the 1st row to be as small as possible. this makes it a good approximation to the 1-D lattice.

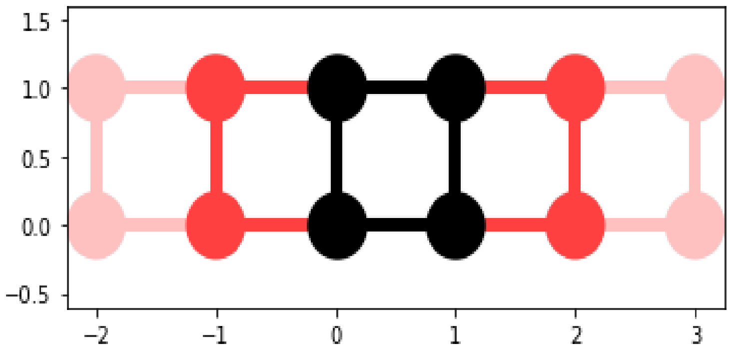
Simulation of 1-D 2-site lattice without scattering

Let us caluclate the conductance through a 1-D 2-Site lattice without any scaterring. Now in the code we have the making of the 1-D lattice with 2-sites.

```
from matplotlib import pyplot
import kwant

# First, define the tight-binding system

sys = kwant.Builder()

# The lattice parameter a
a = 1
lat = kwant.lattice.square(a)

t = 0.5 # t is the coupling stength
W = 2
L = 2

# Define the scattering region

for i in range(L):
for j in range(W):
if j<1:
# On-site Hamiltonian
sys[lat(i, j)] = 4* t
else:
sys[lat(i,j)] = 0



# Hopping in y-direction
if j > 0:
sys[lat(i, j), lat(i, j - 1)] = 0
sys[lat(i,j)]=0
# Hopping in x-direction
```

```
if i > 0:
sys[lat(i, j), lat(i - 1, j)] = -t


# Then, define and attach the leads:

# First the lead to the left
# (Note: TranslationalSymmetry takes a real-space vector)
sym_left_lead = kwant.TranslationalSymmetry((-a, 0))
left_lead = kwant.Builder(sym_left_lead)

for j in range(2):
left_lead[lat(0, j)] =  4 * t
if j > 0:
left_lead[lat(0, j), lat(0, j - 1)] = -0.0001
left_lead[lat(1, j), lat(0, j)] = -t

sys.attach_lead(left_lead)



# Then the lead to the right
sym_right_lead = kwant.TranslationalSymmetry((a, 0))
right_lead = kwant.Builder(sym_right_lead)

for j in range(W):
right_lead[lat(0, j)] = 4* t
if j > 0:
right_lead[lat(0, j), lat(0, j - 1)] = -0.0001
right_lead[lat(1, j), lat(0, j)] = -t

sys.attach_lead(right_lead)

# Plot it, to make sure it's OK
kwant.plot(sys)
# Finalize the system
sys = sys.finalized()
```

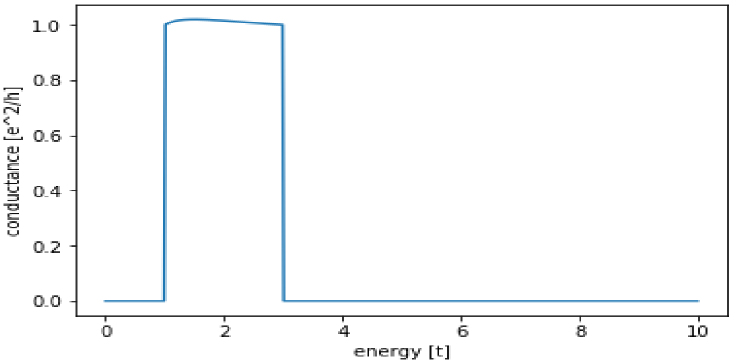
The above code will yield the following lattice



Next we tell the kwant to calculate the conductance fro various values of energy variying in a range

```
# Now that we have the system, we can compute conductance
energies = []
data = []
for ie in range(1000):
energy = ie*0.01

# compute the scattering matrix at a given energy
smatrix = kwant.smatrix(sys, energy)

# compute the transmission probability from lead 0 to
# lead 1
energies.append(energy)
data.append(smatrix.transmission(1, 0))

# Use matplotlib to write output
# We should see conductance steps
pyplot.figure()
pyplot.plot(energies, data)
pyplot.xlabel(”energy␣[t]”)
pyplot.ylabel(”conductance␣[e^2/h]”)
pyplot.show()
```

When this experiment is run we get the following plot



Simulation of 1-D 2-site lattice with scattering

Now we run the experiment with 1 scatterer at 1 site. To achieve this we create the system like the same before

```
from matplotlib import pyplot
import kwant

# First, define the tight-binding system

sys = kwant.Builder()

# The lattice parameter a
```

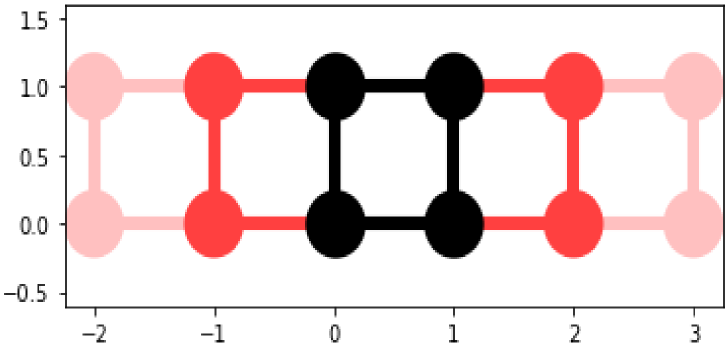
```
a = 1
lat = kwant.lattice.square(a)

t = 0.5 # t is the coupling stength
W = 2
L = 2

# Define the scattering region

for i in range(L):
for j in range(W):
if j<1:
# On-site Hamiltonian
sys[lat(i, j)] =  4* t
else:
sys[lat(i,j)] = 0


# Hopping in y-direction
if j > 0:
sys[lat(i, j), lat(i, j - 1)] = 0
sys[lat(i,j)]=0
# Hopping in x-direction
if i > 0:
sys[lat(i, j), lat(i - 1, j)] = -t


# Then, define and attach the leads:

# First the lead to the left
# (Note: TranslationalSymmetry takes a real-space vector)
sym_left_lead = kwant.TranslationalSymmetry((-a, 0))
left_lead = kwant.Builder(sym_left_lead)

for j in range(2):
left_lead[lat(0, j)] =  4 * t
if j > 0:
left_lead[lat(0, j), lat(0, j - 1)] = -0.0001
left_lead[lat(1, j), lat(0, j)] = -t

sys.attach_lead(left_lead)



# Then the lead to the right
sym_right_lead = kwant.TranslationalSymmetry((a, 0))
right_lead = kwant.Builder(sym_right_lead)

for j in range(W):
right_lead[lat(0, j)] = 4* t
```

```
if j > 0:
right_lead[lat(0, j), lat(0, j - 1)] = -0.0001
right_lead[lat(1, j), lat(0, j)] = -t

sys.attach_lead(right_lead)
```

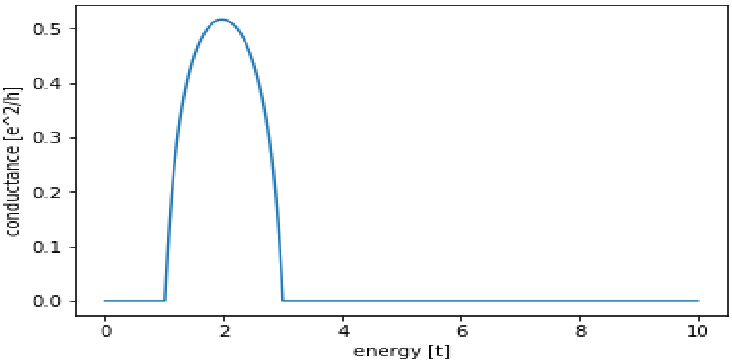
But now we delete a one atom to the right and again introduce the same with a different On-site energy the code for that goes as this

```
del sys[lat(1,0)]
sys[lat(1,0)]=1
sys[lat(0,0),lat(1,0)]=-t
sys[lat(1,0),lat(1,1)]=-0.0001
# Plot it, to make sure it's OK
kwant.plot(sys)
# Finalize the system
sys = sys.finalized()
```

Running the code will yield the following



Now passing this to the kwant to solve for various energies will yeild the following plot



Therefore We find a excellent match between the analytical plots we caluclated in the chapter 8 and the results of the numerical experiments run above. The results are discussed in detail in the next chapter

Here is a generic code that can be used to compute conductance for any 1-D lattice.

```
from matplotlib import pyplot
import kwant
# A code to generate the system
def karthik(n,tau):
# The lattice parameter a
a = 1
lat = kwant.lattice.square(a)
t = tau/2
W = 2
L = n

# Define the scattering region

for i in range(L):
for j in range(W):
if j<1:
# On-site Hamiltonian
sys[lat(i, j)] = 4* t
else:
sys[lat(i,j)] = 0


# Hopping in y-direction
if j > 0:
sys[lat(i, j), lat(i, j - 1)] = 0
sys[lat(i,j)]=0
# Hopping in x-direction
if i > 0:
sys[lat(i, j), lat(i - 1, j)] =-t


# Then, define and attach the leads:

# First the lead to the left
# (Note: TranslationalSymmetry takes a real-space vector)
sym_left_lead = kwant.TranslationalSymmetry((-a, 0))
left_lead = kwant.Builder(sym_left_lead)

for j in range(2):
left_lead[lat(0, j)] = 4 * t
if j > 0:
left_lead[lat(0, j), lat(0, j - 1)] = -0.0001
left_lead[lat(1, j), lat(0, j)] = -t

sys.attach_lead(left_lead)

# Then the lead to the right
sym_right_lead = kwant.TranslationalSymmetry((a, 0))
right_lead = kwant.Builder(sym_right_lead)
```

```
for j in range(W):
right_lead[lat(0, j)] = 4* t
if j > 0:
right_lead[lat(0, j), lat(0, j - 1)] = -0.0001
right_lead[lat(1, j), lat(0, j)] = -t

sys.attach_lead(right_lead)
o=input("press␣y␣if␣you␣want␣scattering␣\t")
if(o=='y'):
coupling=input("Enter␣the␣coupling␣strength␣among␣the␣atoms␣you␣war
coupling=float(coupling)
m=input("Enter␣the␣no␣of␣sites␣of␣scattering␣\t")
m=int(m)
for x in range(m):
site=input("Enter␣the␣site␣index␣(it␣starts␣from␣0)")
site=int(site)
potential=input("Enter␣the␣scattering␣potential")
potential=float(potential)
if(site==0):
del sys[lat(site,0)]
sys[lat(site,0)]=potential
sys[lat(site,0),lat(site+1,0)]=-coupling
sys[lat(site,0),lat(site,1)]=-coupling/10000
elif(site==m-1):
del sys[lat(site,0)]
sys[lat(site,0)]=potential
sys[lat(site-1,0),lat(site,0)]=-coupling
sys[lat(site,0),lat(site,1)]=-coupling/10000
else:
del sys[lat(site,0)]
sys[lat(site,0)]=potential
sys[lat(site,0),lat(site+1,0)]=-coupling
sys[lat(site-1,0),lat(site,0)]=-coupling
sys[lat(site,0),lat(site,1)]=-coupling/10000

else:
print("please␣enter␣correct␣option")
kwant.plot(sys)

# First, define the tight-binding system
sys = kwant.Builder()


n=input("Enter␣the␣value␣of␣n")
n=int(n)
tau=input("Enter␣the␣value␣of␣tau")
tau=float(tau)
karthik(n,tau)
# Finalize the system
```

```
sys = sys.finalized()

# Now that we have the system, we can compute conductance
energies = []
data = []
for ie in range(1000):
energy = ie*0.01

# compute the scattering matrix at a given energy
smatrix = kwant.smatrix(sys, energy)

# compute the transmission probability from lead 0 to
# lead 1
energies.append(energy)
data.append(smatrix.transmission(1, 0))

# Use matplotlib to write output
# We should see conductance steps
pyplot.figure()
pyplot.plot(energies, data)
pyplot.xlabel("energy␣[t]")
pyplot.ylabel("conductance␣[e^2/h]")
pyplot.show()
```

Chapter 10

RESULTS AND FURTHER WORK

Results are analysed here in three divisons

1. Results of conductance of a 1-D lattice without scattering
2. Results of 1-D lattice of a 1-D lattice with scattering
3. Results of conductance of a 1-D lattice with more than 1 scattering

10.1 Results of conductance of a 1-D lattice without scattering

The conductance of lattice without scattering is basically a constant and the amplitude of the conductance purely depends only on the strength of the onsite potential. If the potential is really high then the conductance ofcourse will go down and also the allowed values of energy as per the relation 8.10 will also go down, this will also narrow the curve. Therefore in a solid of really high onsite potential like that of alkali or alkaline metals only a narrow range of energy values are allowed for a conduction from that channel.

10.2 Results of conductance of a 1-D lattice with scattering

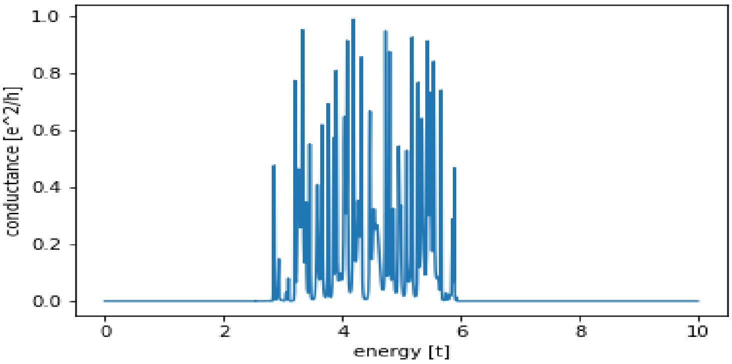
Now the scatterer is like the impurity or a defect in the crystal. this hinders or disturbs the incoming electron and hence it affects the conductance and that is the reason we see a drop in the amplitude (dropped by half the initial value) of the conductance in the fig 9.3. In this context we neglect the electron electron collision and interaction

10.3 Results of conductance of a 1-D lattice with more than 1 scatterer

In the real world we find all solids with defects and impurity and in a non-ideal solid there might be imourities that are random at sites as well as potentials too hence there would be more than 1 scatterinig that would happen in a real solid. In that case the intution says that as the no.of scatterers increases the conductivity should go down but strangely if there are finite and considerably less amount of impurity we experimentally find there are absolute transmission at some energy values which is totally against the classical picture.

This is where the quantum mechanical methods such as the NEGF method solves the issue. In the whole of our discussion we have taken the electron to be a wave and we know that the waves interfere to form maximum and minimum the same phenomena happens in the case of the transmission and at specific values of the energy we find maximum conductance.

The result of a 1-D lattice with 100sites with random scattering is as follows



10.4 FURTHER WORK

In this work we have asumed that there exist only 1 source and a drain term basically its a 1-channel problem but in real solids when it is connected to a source then a band of channels are created and one can also analyse that. It would just be a summation of all the effects but with some suttle aspects to be taken care of (like the total probability current will be summed up individually)

Similarly we have in the example worked out only for the 1-D lattice but Kwant usually can calculate for a N-D lattice too. The analytics will be much harder to compute in that case.

Using kwant one can also calculate various parameters like the Local Density of States and the Greens function corresponding to the different operators.

My further Work is inteded in extending to the 2-D lattice and also to irregular lattices like Graphene . I also intend to calculate the Local Density of States of such a 2-D system at various energies.

$$G = (E - \epsilon_k + i\delta)^{-1} \tag{10.1}$$

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