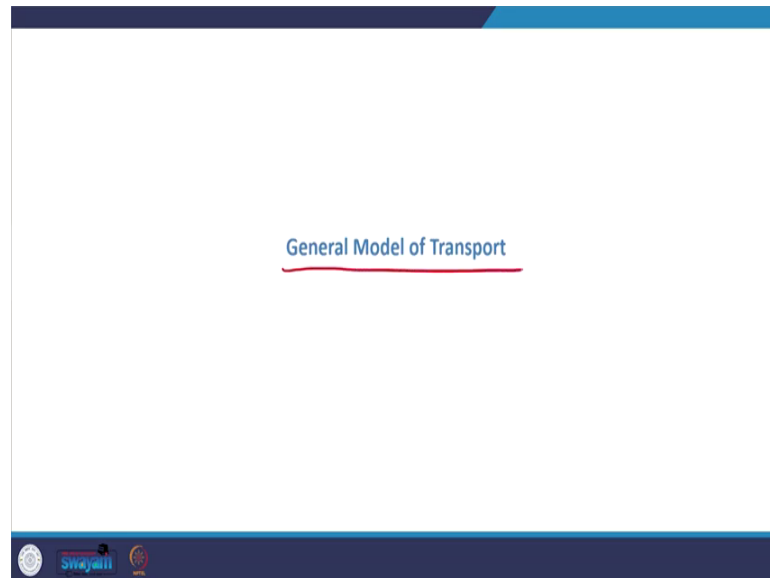


Physics of Nanoscale Devices
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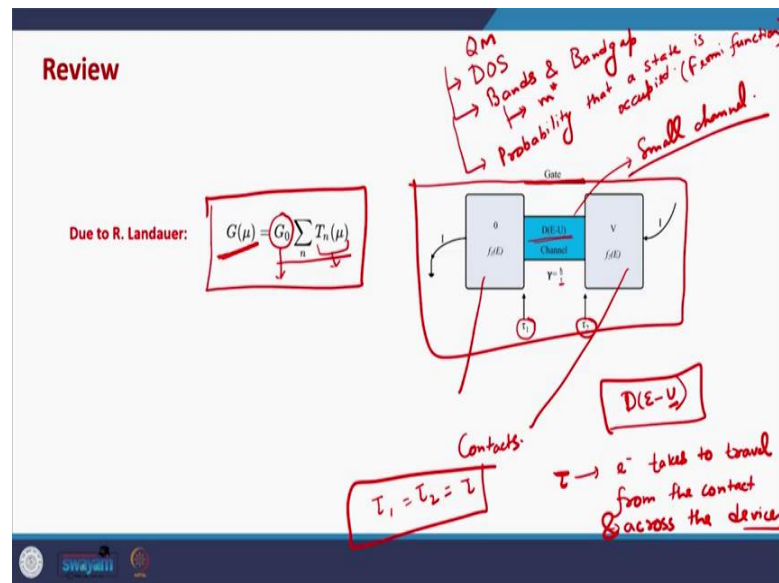
Lecture - 18
General Model of Transport - II

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Hello everyone. Today we will continue our discussion of the General Model of Transport and as all of you know from last class on we started discussing how electrons actually travel through devices.

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So, after building a background of basics of quantum mechanics then from quantum mechanics we saw how density of states which means how allowed electronic energy states in a system are obtained. So, we obtain the notion of density of states, we understood the notion of bands and band gaps in solid.

And in addition to this we also saw that when the EK diagram is parabolic diagram then this can be. So, this quantum mechanical formulation can be sort of and specially the influence of a applied force can be modeled pretty much like a classical system and in that we need to take effective mass of the electron instead of the simple mass. Then we saw the probability that state is occupied or not and that is given by the Fermi functions. So, we also went through the notion of Fermi function and an allied notion of Fermi level.

So, with these ideas, we started discussing the transport and specially the transport in mesoscopic devices. Mesoscopic means they are not of atomic dimensions, but they are few times of nanometers which is actually the dimension of transistors in 2020 or even now a days ok. So, this formalism of electron transport in devices was originally given by Landauer and according to Landauer the electrical conductance of a conductor is given by this formula where on the left hand side we have the conductance.

On the right hand side this G_0 is a constant is known as the quantum of conductance and these $T_n(\mu)$ are known as the transmission eigen values of electrons and n denotes various channels of the electrons in a device. So, essentially according to Landauers formalism the

total conductance of a material is the sum of conductance or sum of transmission possibilities in various channels in a device, multiplied by a fundamental constant which is known as the quantum of conductance.

So, this formalism was further, I would say generalized and sort of it was reformulated by Professor Supriyo Datta and professor later Professor Mark Lundstrom and that is what we will study here. The system of interest to us is a two terminal device, a device like this in which we have a small channel in between two large contacts. So, there are two contacts and there is a small channel in between. The contacts are characterized by the Fermi functions of those contacts and the channel is characterized by the density of states in the channel ok. The density of states is a function of energy.

So, the allowed energy states depend on the energy at which we are sort of interested in. In addition to that there might be various interactions that the electron might be undergoing. So, when an electron travels through a device, it might interact with other electrons in addition to that we might have a gate like structure where we can apply a voltage and we can produce an electric field in the channel and that will modify the potential energy of the electron.

So, this density of states in the channel is written as $D(E - U)$ essentially. Where, U is the potential because of the other interactions or because of the potential energy of the electron because of its interaction with other particles in the surrounding. Or it is, it might be the modification in energy of electrons because of the voltage applied on the third terminal the gate terminal essentially.

So, in addition to these things we have another parameter here known as the characteristic time, characteristic time τ which essentially in a way models the interaction or the connection of the contact to the channel. So, τ is the time that the electron takes from the contact to travel through the device. So, the τ is the time that electron takes to travel from the contact across the entire device and across the device. So, when the when this channel is long in that case τ essentially will become the transit time of electron, τ becomes or τ is dominated by the time that the electron takes to travel through the long channel.

So, in long channel generally the time that it takes to, it takes for the electron to hop from the contact to the channel is negligible as compared to the time that the electron takes to travel through the channel ok. So, for long channels it essentially becomes the transit time

or the travel time of electrons through the channel for short channels even for short channels the time that the electron takes to jump from the contact to the channel.

And that is also significant as compared to the time that the electron takes to travel through the channel and there we need to consider both the times. The time that the electron takes to jump from the channel to the, from the contact to the channel and to travel through the channel ok. So, finally, we have very simple parameters I would say. The Fermi functions of the contacts the density of states of the channel and the characteristic time of the contact and the channel.

So, if the contacts are different these characteristic times are different τ_1 corresponding to contact 1 or the source contact. τ_2 corresponding to contact 2 or the drain contact ok. Generally, in most of our devices both the contacts are identical and in that case τ_1 is equal to τ_2 is equal to τ ok.

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General model of transport

Most important: channel – described by $D(E-U)$

U – electrostatic potential [can be manipulated by gate]

Contacts: large regions, described by the Fermi function:

$$f_0 = \frac{1}{1 + e^{(E-E_F)/k_B T_L}}$$

T_L – Lattice temperature

Handwritten notes:

- ① Electronic Population (charge) in the channel in Steady State.
- ② Current in the device (I-V characteristics)

Energy level diagram:

- Labels: E_{FS} , E_{FD}
- Labels: E_{FS} , E_{FD}
- Labels: $\Delta E \cdot \Delta t = k$, $\Delta E = \frac{\hbar}{\tau}$
- Equation: $\gamma = \frac{k}{\tau}$
- Label: Energy

Diagram: A schematic of a quantum dot or channel with two contacts (0 and V) and a gate. It shows current I and characteristic times τ_1 and τ_2 . A red arrow labeled "Inelastic scattering" points to the channel. A red arrow labeled "Steady State" points to the channel. A red arrow labeled "Near Equilibrium State" points to the contacts.

So, with these things we will essentially start our discussion on how electrons travel through the device and what could possibly be the expression of the current through the device. So, that is essentially what we want to finally, find out we want to finally, find out the I-V characteristics of the device.

Which means what would be the current through the device when we apply a certain voltage across the device. A related concept here is the concept of γ . So, when the channel

is very small, as we know by now that in very small channels the energy levels will be discrete because the confinement leads to discretization. And in these discrete energy levels, electrons only spend in total time τ , right from coming from the contact to travel through the channel.

So, according to the Heisenberg's uncertainty principle there will be a certain energy uncertainty in these energy levels, because the finite because the electron spends finite life time in the in these energy levels. And the broadening in energy ΔE will be governed by the Heisenberg's uncertainty principle.

So, ΔE and we are taking the lower limit of the of the Heisenberg's uncertainty principle, Δt is essentially τ ; τ is the time that the electron spends on an average in the channel. And this is defined as another parameter $\Upsilon = \frac{\hbar}{\tau}$. So, Υ is essentially an energy quantity, it has units of energy it corresponds to the broadening of energy levels in the channel because of the finite life time of electrons in small devices.

So, now we are all set to sort of start seeing how electrons travel through the device and as I discussed in previous classes that when there is no net transport of electrons through the device the device is said to be at equilibrium. So, equilibrium is the state when every process is balanced by the reverse process. So, every flow of electron is balanced by the reverse flow of electrons; however, when we apply a certain voltage that will create a difference in the Fermi levels of the source and the drain.

And because of the difference in the Fermi levels of the source and the drain. There will be, I would say an imbalance in electron population on the source side and on the drain side and that will create or that will start a flow of electrons from the source to the drain. And if that voltage difference is maintained by a battery in the device, this state will be there we will achieve a constant current in the device after a small time.

So, this state when the flow is constant in a system that is known as the steady state and there is an important sort of, I would say observation that we need to make here or even we can say it approximation that the contacts are large and electrons undergo inelastic scattering in the contacts.

What it means is that electrons energy is not preserved during collisions when they collide with each other or with the other atoms in the contacts. And what that essentially amounts

to is that whatever be the applied voltage ultimately very quickly electrons distribution because of the inelastic scattering becomes very close to the equilibrium distribution ok.

So; that means, that contacts are always in near equilibrium state ok. So, even with an applied voltage contacts maintain a near equilibrium state which means that electronic distribution in the contacts can still be given by the Fermi functions and the Fermi level. And because the contacts are large, even if some electrons go from contacts to the channel or some electrons come from channel to the contact it will not change the population of electrons significantly in the contacts.

Because already there is a huge population of electrons in the contacts and no significant change in population takes place because of the electron flow, that essentially means is that the Fermi levels in the contacts are constant. The Fermi level of the source contact generally denoted as E_{FS} and or the Fermi level of the drain contact generally denoted as E_{FD} , they are almost always constant because of the near equilibrium situation in the contacts during transport ok.

So, these are a couple of things; however, since the channel is small and the number of electrons that exist in the channel will; obviously, be small as compared to the contacts. So, when the channel is put in between the contacts the number of electrons in the channel might change significantly. So, what it means is that the electronic population in the channel can change significantly and that is also an important quantity or important parameter that we need to understand in the transport, what is the steady state electronic population or steady state charge in the channel.

So, there might be certain population of electrons or certain number of electrons in the channel before contacts are put on and voltage is applied. But when contacts are put and a voltage is applied the electronic population in the channel is modified significantly and that is also what we would like to understand. So, we would like to understand two things essentially, one is the electronic population or charge in the channel in steady state and 2nd is we would like to understand the current or current in the device or I-V characteristics, current in the device or I-V characteristics ok.

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General model of transport

Most important: channel – described by $D(E-U)$

U – electrostatic potential [can be manipulated by gate]

Contacts: large regions, described by the Fermi function:

$$f_0 = \frac{1}{1 + e^{(E-E_F)/k_B T_L}} \quad T_L - \text{Lattice temperature}$$

No Voltage: $E_{F2} = E_{F1}$

With Voltage: $E_{F2} = E_{F1} - qV$

Contact to channel connection: τ In energy units: $\gamma = h/\tau$

For single molecule: energy broadening.

Three important parameters: DOS, Fermi levels, Transit time (characteristic time for contact and channel)

The diagram illustrates a two-terminal device with source (S) and drain (D) contacts and a central channel. A gate is positioned above the channel. The diagram shows energy levels E_{FS} and E_{FD} , and electronic states in the channel. Handwritten notes include $V_D = 0$ Equilibrium and Electronic States in Channel.

So, without any further delay let us see what happens. These are two contacts this is source, let us say this is drain, this is channel in between and for the moment let us say the gate is not there, this is not there we only have a two terminal device the source, the drain and the channel. When there is no voltage applied and the source and the drain contacts are identical in that case the Fermi levels of the source and the drain E_{FS} and E_{FD} are at the same level and there might be.

So, the allowed electronic states in the channel is governed by the or is given by the density of states and the band structure of the channel. So, this could possibly be one of the electronic state configuration of the channel, electronic states in the channel. So, this is the situation when there is no externally applied voltage on the device. V applied is 0 or V drain is 0, generally the source is kept at grounded and kept grounded and V apply a battery at the drain terminal ok.

So, in this case nothing happens in the device because both the contacts Fermi level are at the same level. So, no net electron flow is there and this situation is the equilibrium of the device essentially. But as soon as we apply a voltage on the drain terminal, as soon as we connect a battery across the source and the drain that will essentially bring down the drain Fermi level.

So, that will and this we have seen multiple times by now, that now the drain Fermi level let us say will come down to this energy level E_{FD} is here and this is the equal to q times

V_D . Where, V_D is the drain applied drain voltage. Now, what will happen is that this contact, the source contact will try to bring the channel in equilibrium with itself; what does that mean? That means, that it will try to fill all electronic states up to its Fermi level in the channel.

And since the contact is large, even if some electrons hop or jump from source into the channel it does not create any difference for the source contact ok. So, it will try to bring the channel in equilibrium with itself. Similarly, the drain contact will also try to bring the channel in equilibrium with itself. And what does that mean? That means, that it will try to make sure that all the energy levels in the channel up to its Fermi level E_{FD} are filled.

So, all the energy levels up to this point are filled, this is what this the drain contact will try to make sure. What does that mean? That it means, that the energy levels above E_{FD} for those energy levels if there are electrons in those energy levels in the channel, it will try to make sure that it is the these those energy levels are empty.

It will try to make sure that electrons are not there in the energy levels above its Fermi level. So, essentially E_{FS} is trying to fill all electronic states up to this point, E_{FD} is trying to fill all the electronic states up to this point. And it will try to empty all the electronic states above E_{FD} that will essentially create a flow of electrons from E_{FS} to E_{FD} .

So, electrons will go from here to here, from here to here and all the electronic states below E_{FD} will be filled. So, all these electronic states will be filled in any case ok. So, this is how a current will be maintained in the system.

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General model of transport

Handwritten: $D(E) = g_{sp}(E) \cdot V = g_{sp}(E) \cdot A \cdot L$

Questions:

- How is the electron density in the device related to the DOS, Fermi levels, and characteristics times.
- Expression for the current.

The Model

Left contact will seek to fill up the states in the channel according to E_{F1} . At equilibrium between channel and left contact, number of electrons between E and $E + dE$:

$$N'_1(E)dE = D(E)dE f_1(E)$$

Handwritten: $N'_1 = D(E) \cdot f_1(E) dE$
↳ Fermi function of source contact

Now, let us look at this situation differently. Now, let us say that this is source, this is drain, this is channel these are various allowed electronic states in the channel ok, E_{FS} is up to this point, E_{FD} is up to this point alright. So, in equilibrium for the moment let us assume that the channel is just in contact with the source. So, we only have source and channel in contact with each other, in that case as I told that this since the source contact is large. So, it will try to bring the channel in equilibrium with itself with the source contact.

So, what it means is that it will try to fill all electronic states in the channel up to its Fermi level. So, then in equilibrium when the source is in equilibrium with the channel the number of electrons between energy E and $E + dE$ in a small energy range of dE will be. So, let us say this is number of electrons, this is the energy range dE ok.

So, the number of electrons in this small interval of energy will be given by let us denote it by N'_1 , this will be given by the density of states in the channel. Number of electrons is essentially density of states into the probability of the states getting occupied $f_1(E)$ into energy range. So, where $f_1(E)$ is the Fermi function of the source contact. So, it is as if the source contact is trying to fill all electronic states according to its Fermi function ok. So, that is in other terms is the state of equilibrium between the source and the channel.

So, when we assume that only source is connected to channel this would be the number of electrons in the energy range E to $E + dE$ in the channel and this is governed by the density

of states in the channel times the Fermi function of the source times the energy range. And please keep in mind here, this density of states here is since we are trying to calculate the total number of electrons in the channel. This is the density of states that we calculated earlier times volume for 3D channels, it is $g(E)$ for 3D channels it is g_{3D} into volume, for 2D channels it is g_{2D} into area and for 1D channels it is g_{1D} times length.

So, this is in a way the number of allowed electronic states in the entire volume of the 3D channel or for a 2D channel this is the number of electronic states in the entire area or for 1D channel it is the number of allowed electronic states in the entire length ok. So, this is the case when only the source contact is connected to the channel. Now, let us assume that only the drain contact is connected to the channel and in the same sort of line of arguments the drain contact will try to bring the channel in equilibrium with itself.

So, it will try to fill the channel states according to the Fermi function of the drain and if the Fermi function of the drain is $f_2(E)$, Fermi function of the source is $f_1(E)$.

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General model of transport

Questions:

- How is the electron density in the device related to the DOS, Fermi levels, and characteristics times.
- Expression for the current.

Handwritten notes:

$D(E) = g_{3D}(E) \cdot V$
 $= g_{2D}(E) \cdot A$
 $= g_{1D}(E) \cdot L$

In steady state:
 The no. of e^- in the channel is N'

The rate at which e^- are going from source \rightarrow right through the channel:-
 $F_1 = \frac{N'_1 - N'_2}{\tau_1}$

Drain to channel $\rightarrow F_2 = \frac{N'_2 - N'_1}{\tau_2}$

$N'_1 = D(E) \cdot f_1(E) \cdot dE$
 $N'_2 = D(E) \cdot f_2(E) \cdot dE$

In equilibrium when the channel is only connected to the drain contact in that case the number of, let us say in equilibrium the number of electrons in the channel is N'_2 . And that will be the density of states of electrons in the channel times the Fermi function of the drain times the energy range dE .

So, N'_1 is the number of electrons in energy range E to $E + dE$ when the channel is only connected to source. N'_2 is the number of electrons be in the energy range E to $E + dE$ when the channel is only connected to the drain contact. But in our two terminal device, please ignore this gate terminal here, for the moment let us assume that the third terminal is not there and we only have a two terminal device. In the two terminal device both contacts are connected simultaneously.

So, the electronic population in the steady state. So, if the, this E_{FS} and E_{FD} are different levels in that case there will be a net flow of electrons and the number of electrons in the channel will be slightly or will be somewhat lesser than N'_1 and somewhat more than N'_2 . Because this is trying to make sure that N'_1 electrons are there in the channel, essentially all the states up to this point are filled.

The drain contact is trying to make sure that N'_2 electrons are there in the channel up to this point states are filled. In steady state when both contacts are connected the electronic population will be somewhat in between N'_1 and N'_2 . So, let us say that in steady state, the number of electrons in the channel is N' ok. So, in that case we now know what is the source contact trying to do, it is trying to maintain N'_1 electrons.

It is continuously sort of pumping electrons in the channel so that electronic population becomes N'_1 , the drain contact is trying to make sure that N'_2 electrons are there in the channel. It is continuously taking electrons out of the channel so that only N'_2 electrons are there. In steady state N' electrons are there.

Now, we can write the rate at which electrons are going from the source into the channel or through the channel. So, the rate at which electrons are going from source right through the channel is if this rate is denoted as F_1 , this will be essentially $N - N'$ divided by τ_1 .

Because one electron is taking on an average time τ_1 to go from source right through the channel. So, this is the rate at which the source will be pumping electrons into the channel. And similarly, the rate at which from drain to channel let us say, electrons will be going from drain to channel if that is denoted as F_2 will be $N'_2 - N'$ by τ_2 . And as we intuitively know that this N'_2 is less than N' so this rate will be negative.

And what it means is that electrons are going from the channel to the drain and not in from the drain to the channel. So, these are the rate equations in this model. Now, just take a

moment and think what will happen in steady state and that is where we will begin our discussion in the next class from ok.

So, with simple sort of understanding of the Fermi functions, the density of states, the characteristics time we have written the rate equations or the rate at which electrons will be flowing from the source to the channel or from the channel to the drain. With this we would be able to find out two parameters that we are interested in, one is the steady state population of electrons in the channel and second is the current through the device and that is what we will do in the coming class.

Thank you for your attention see you in the next class.