

Physics of Nanoscale Devices
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Lecture - 23
Modes, Diffusive Transport

Hello everyone, today we will discuss the idea or I would say we will finish the concept of modes in a device and we will start a new topic the topic of Diffusive Transport. So, please remember that the transport that we studied in last few classes was ballistic transport, which means that the electron that was starting from the source side was directly going to the drain side. There was no collision in between, no energy loss or no such kind of things was happening in the device.

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Review

$$N = \int \frac{D(E)}{2} (f_1 + f_2) dE$$

$$I = \frac{2q}{h} \int \gamma(E) \pi \frac{D(E)}{2} (f_1 - f_2) dE = \frac{2q}{h} \int M(E) (f_1 - f_2) dE$$

1D: $D(E) = D_{1D}(E)L = \frac{L}{\pi\hbar} \sqrt{\frac{2m^*}{(E - E_c)}} H(E - E_c)$

2D: $D(E) = D_{2D}(E)A = A \frac{m^*}{\pi\hbar^2} H(E - E_c)$

3D: $D(E) = D_{3D}(E)\Omega = \Omega \frac{m^* \sqrt{2m^*(E - E_c)}}{\pi^2\hbar^3} H(E - E_c)$

$$E(k) = E_c + \hbar^2 k^2 / 2m^*$$

$$v_x(k) = \frac{1}{\hbar} \frac{\partial E}{\partial k} = \frac{\hbar k}{m^*}$$

Diagram: A schematic of a device with source and drain electrodes. The source is at energy E_1 and the drain is at energy E_2 . The device length is L . Fermi functions $f_1(E)$ and $f_2(E)$ are shown at the electrodes. A coordinate system (x, y, z) is centered in the device. A red arrow indicates the direction of transport.

Mode expressions:

- 1D: $M(E) = M_{1D}(E) = H(E - E_c)$
- 2D: $M(E) = WM_{2D}(E) = W \frac{\sqrt{2m^*(E - E_c)}}{\pi\hbar} H(E - E_c)$
- 3D: $M(E) = AM_{3D}(E) = A \frac{m^*}{2\pi\hbar^2} (E - E_c) H(E - E_c)$

Before going into the diffusive transport case let me quickly review what we have covered so far. So, we have seen in our discussion of general model of transport that in equilibrium the electrons in the device are in a steady state, not in equilibrium because when the current is flowing this is the steady state situation. The steady state number of electrons in the device is given by this expression and the steady state charge will be just q times this.

And the steady state current in the device is given by this expression which can further be rewritten as $\frac{2q}{h} \int M(E)(f_1 - f_2)dE$ ok. We already have derived these expressions, these

are just expressions from the density of states. The D here is the density of states times volume for 3D materials, 3D channel area times density of states in 2D channel and length times density of states in 1D channel.

And that is what is shown here, we have for the electrons that are undergoing transport, we have discussed that most of those electrons are the electrons very close to the bottom of the conduction band and in that situation this parabolic relationship between E and k holds true.

So, E is equal to $E_c + \frac{\hbar^2 k^2}{2m^*}$ and the average velocity in x direction which essentially appears and which is crucial for calculation of modes is given by this expression. And by using this velocity expression and the number of electronic states per unit energy expression we can derive the expressions for the modes in the device.

And this is what it turns out to be for 1D channel device for 2D channel device and this is for the 3D channel device, please keep in mind I would just remind you that this H function here is the step function Heaviside step function. So, the form of this function is something like this.

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Review

$$N = \int \frac{D(E)}{2} (f_1 + f_2) dE$$

$$I = \frac{2q}{h} \int \gamma(E) \pi \frac{D(E)}{2} (f_1 - f_2) dE = \frac{2q}{h} \int m(E) \cdot (f_1 - f_2) \cdot dE$$

1D: $D(E) = D_{1D}(E)L = \frac{L}{\pi\hbar} \sqrt{\frac{2m^*}{E - E_c}} H(E - E_c)$

2D: $D(E) = D_{2D}(E)A = A \frac{m^*}{\pi\hbar^2} H(E - E_c)$

3D: $D(E) = D_{3D}(E)\Omega = \Omega \frac{m^* \sqrt{2m^*(E - E_c)}}{\pi^2 \hbar^3} H(E - E_c)$

$$E(k) = E_c + \hbar^2 k^2 / 2m^*$$

$$v_x(k) = \frac{2}{\pi} v = \frac{2}{\pi} \sqrt{\frac{2(E - E_c)}{m^*}}$$

H(E - E_c)

⇒

$E < E_c$ E_c E

The diagram shows a schematic of a device with length L and width W, with energy bands E₁ and E₂ and chemical potentials μ₁(E) and μ₂(E). A coordinate system (x, y, z) is shown. The Heaviside step function H(E - E_c) is plotted as a function of energy E, showing a step at E_c.

A Heaviside step function, let us say H(E - E_c) will have this kind of form. If this is the energy axis and if this is on the y axis we have H(E - E_c). So, this function will be 0 before energy E_c and this will be 1 at energy E_c. So, this will be the form of the Heaviside step

function 0 to 1 ok, which means that generally so these expressions will be 0 before E equal to Ec.

Because this introduces a factor of 0 before E equal to Ec, for this energy range this all these expressions are 0. So, it means that we are talking about or we are only interested in the conduction band of the devices ok. Similarly, in the expression for the number of modes.

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Review

$$N = \int \frac{D(E)}{2} (f_1 + f_2) dE$$

$$I = \frac{2q}{h} \int \gamma(E) \pi \frac{D(E)}{2} (f_1 - f_2) dE.$$

1D: $D(E) = D_{1D}(E)L = \frac{L}{\pi\hbar} \sqrt{\frac{2m^*}{E - E_c}} H(E - E_c)$

2D: $D(E) = D_{2D}(E)A = A \frac{m^*}{\pi\hbar^2} H(E - E_c)$

3D: $D(E) = D_{3D}(E)\Omega = \Omega \frac{m^* \sqrt{2m^*(E - E_c)}}{\pi^2\hbar^3} H(E - E_c)$

$$E(k) = E_c + \hbar^2 k^2 / 2m^*$$

$$v_g^*(E) = \frac{2}{\pi} = \frac{2}{\pi} \sqrt{\frac{2(E - E_c)}{m^*}}$$

$M(E) = M_{1D}(E) = H(E - E_c)$

$M(E) = WM_{2D}(E) = W \frac{\sqrt{2m^*(E - E_c)}}{\pi\hbar} H(E - E_c)$

$M(E) = AM_{3D}(E) = A \frac{m^*}{2\pi\hbar^2} (E - E_c) H(E - E_c)$

Handwritten formula: $M(E) = \frac{W}{(\lambda_B/2)}$

Diagram: A schematic of a device with length L and width W. It shows two electrodes with Fermi levels $E_{F1}(E)$ and $E_{F2}(E)$. A coordinate system (x, y, z) is shown with the x-axis along the device length and the y-axis along the width. A red arrow indicates the direction of electron flow.

Apart from this there is a very intuitive explanation of what is modes specially in a 2D channel, in a 2D channel we explicitly derived it this is essentially the ratio between the width and the half de Broglie wavelength of the electrons.

So, this is the number of modes is the number of half wavelengths of the electrons that can fit into the width of the device and similarly in a 3D device it will be essentially the number of half wavelengths that can fit in the cross section of the device.

And in 1D device it has a different connotation according to this expression. Specially in 1D device as you can see this is essentially constant, because there can be only I would say 1 mode in the 1D device, 1 conduction pathway for the electrons.

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Modes for 1D, 2D and 3D

DOS: 1D: $D(E) = D_{1D}(E)L = \frac{L}{\pi\hbar} \sqrt{\frac{2m^*}{(E - E_c)}} H(E - E_c)$ $g_{1D}(E) = D_{1D}(E) \propto \frac{1}{\sqrt{E - E_c}}$

2D: $D(E) = D_{2D}(E)A = A \frac{m^*}{\pi\hbar^2} H(E - E_c)$

3D: $D(E) = D_{3D}(E)\Omega = \Omega \frac{m^* \sqrt{2m^*(E - E_c)}}{\pi^2\hbar^3} H(E - E_c)$

$E(k) = E_c + \hbar^2 k^2 / 2m^*$

$v_g(E) = \frac{2}{\pi} v = \frac{2}{\pi} \sqrt{\frac{2(E - E_c)}{m^*}}$

Corresponding modes:

$M(E) = M_{1D}(E) = H(E - E_c)$, $M(E) = 1, E > E_c$

$M(E) = W M_{2D}(E) = W \frac{\sqrt{2m^*(E - E_c)}}{\pi\hbar} H(E - E_c)$

$M(E) = A M_{3D}(E) = A \frac{m^*}{2\pi^2\hbar^3} (E - E_c) H(E - E_c)$

So, now with these expressions at our hands we are now in a situation to compare the 2 important quantities in conduction and transport of electrons in devices, one is the density of states which is represented as D_{1D} , D_{2D} or D_{3D} and second is the number of modes in the same channel. So, as you can see that for let us say for 1D device, for 1D device the density of states which is essentially $g_{1D}(E)$ also written here as $D_{1D}(E)$ is inversely proportional to the energy.

And the number of modes this $M(E)$ is constant for the 1D channel $M(E)$ is essentially 1 for E greater than E_c . So, this number of modes is constant in 1D device and the density of states is a decreasing function, very quickly decreasing function and as you might have seen and we have already discussed this that the density of states in 1D device has the maximum value close to the bottom of the conduction band.

So, which means that if these are the edges of the conduction and valence band in the channel, if the channel is very small we cannot define bands as we define in the bulk material.

But we can define still there are regimes or still there are highest occupied molecular orbitals or highest occupied states and lowest unoccupied states and those states will be equivalent to the valence band and the conduction band in the bulk materials ok.

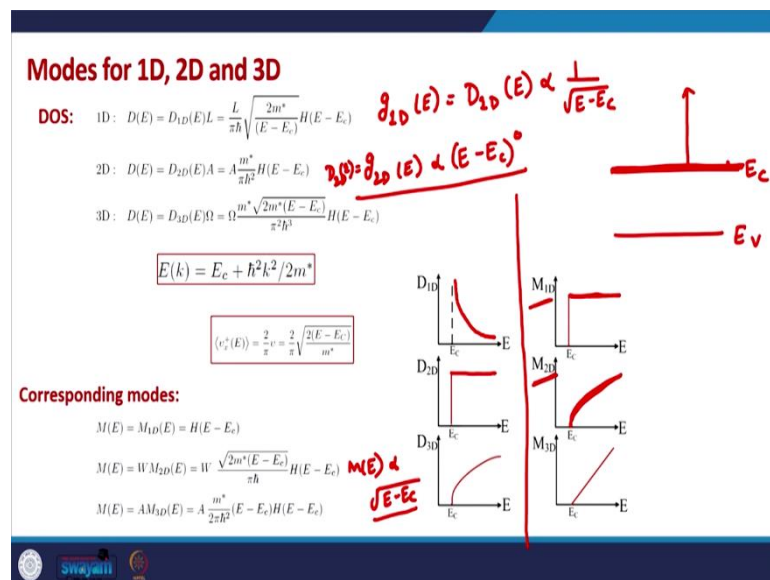
So, we saw that the density of states is maximum at the bottom of the conduction band in a 1D material, it has the maximum value tends to almost infinity at the bottom of the conduction band. So, which means that most of the available electronic states in a 1D

channel are actually close to the bottom of the conduction band almost all the available electronic states are the at the bottom of the conduction band.

But that is not the case with number of modes as we might tend to think that modes and density of states are almost similar concepts they are correlated to each other, but they are qualitatively and physically they are quite different.

Number of modes; however, is constant as a function of energy it is only at all energy levels above the bottom of the conduction band, the number of modes is a constant 1. There is only 1 mode which is available for the electron to transfer transport ok.

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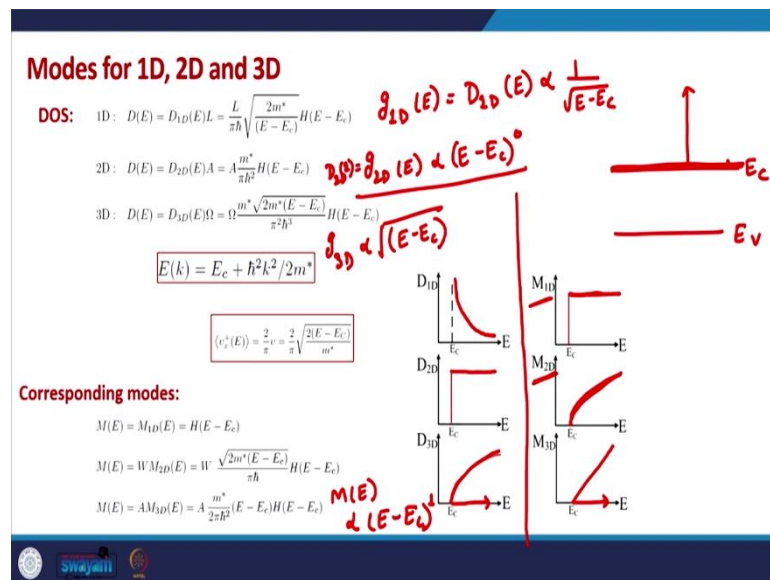
In a 2D device in a 2D channel, a device which has a 2D channel as is clear from the expressions that density of states is directly is constant essentially, it is independent of the energy, proportional to $E - E_c$ to the power 0. Whereas, the modes in a 2D channel is directly proportional to the square root of $E - E_c$, what it implies is that if we plot density of states g_{2D} or $D_{2D}(E)$.

It will be constant as a function of energy in a 2D channel. Whereas, the number of modes in the channel will be an increasing function. So, it will be something like this $M(E)$ versus E will be something like this, it means that the density of states the number of available electronic states in the device is constant for all energy levels after the bottom of the conduction band.

Whereas, the number of modes in the channel is very small close to the bottom of the conduction band almost 0 which means that, while traveling through the device while electrons are transporting through the device from the source to the drain number of pathways available close to the bottom of the conduction band is very small almost 0. And the number of conduction pathways increases in number as we go away from the bottom of the conduction band.

So, as you can see here physically these two notions are very different although they are highly correlated with each other, they are actually this number of modes the notion of modes comes from the notion of density of states and the energy broadening, but physically it is quite different than the density of states as is also clear in the 2D channel.

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And similarly in a 3D channel, if we look at the expressions, the density of states in a 3D channel is directly proportional to the square root of $E - E_c$. Whereas, the number of modes in a 3D channel is directly proportional to the $E - E_c$ to the power 1/2.

So, what it means is that in a 3D channel both density of states and modes are increasing function as we increase the energy beyond the bottom of the conduction band, after the energy E_c both are increasing function.

But the way they increase is different. In first case it is a square root dependence and in second case it is a linear dependence ok. So, this is the comparative study of density of

states and the idea of modes in a device. So, please keep in mind that this idea of modes is a very important idea and physically it has important connotation when we talk about current.

Because in while the current is flowing, while there is a steady state flow of electrons in the device in that case it tells us about the number of conduction pathways as a function of energy in the device. So, with this we are in a position to basically summarize the discussion of modes in few points.

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Modes - In summary

- The density-of-states vs. E is used to compute carrier densities. ✓
- The number of modes (channels) vs. E is used to compute the current.
- The number of modes at energy, E, is proportional to the average velocity (in the direction of transport) at energy, E, times the density-of-states, D(E).
- M(E) depends on the band structure and on dimensionality.

$$N = \int D(E) \cdot \frac{(f_1 + f_2)}{2} dE$$

$$I = \frac{2e}{h} \int M(E) \cdot (f_1 - f_2) \cdot dE$$

I-V characteristics

$$M(E) = \gamma(E) \cdot \pi \cdot \frac{D(E)}{2}$$

$$\gamma(E) \propto \frac{1}{v(E)} \propto \frac{\langle v_x^2(E) \rangle}{L}$$

The density of states versus E is used to compute the carrier density. Because as we can recall from this expression the relationship between the carrier density or the steady state electron population in the device is this.

So, while we are interested in calculating the density the carrier densities number of charge carriers in a device, we need the relationship between dE and E and we integrate that plot with a multiplication factor of $\frac{f_1 + f_2}{2}$. Similarly, the expression for the current is this it is basically $f_1 - f_2$ times M(E) times dE.

So, the relationship between M(E) and E and the integration of the plot of M(E) versus E with a factor of multiplication factor of $f_1 - f_2$ gives us the current in the device. And this is an important expression because this also gives us the I-V relationship I-V

characteristics of any arbitrary device. The number of modes at any energy E is proportional to the velocity as we have already seen.

Because this factor of $\gamma(E)$ number of modes at any energy is equal to $\frac{\gamma\pi D(E)}{2}$ and this factor of $\gamma(E)$ is inversely proportional to $\tau(E)$ and $\tau(E)$ is further inversely proportional to average velocity. So, it makes $\gamma(E)$ directly proportional to average velocity ok.

So, it is the average velocity times the density of states of electrons in the device, that is what determines the number of modes and as we have seen that $M(E)$ depends on the band structure and on the dimensionality. Band structure means the $E-k$ relationship ok, because the $E-k$ relationship will govern the density of states, it will also have an impact on the $\gamma(E)$ the energy broadening and that will further determine the number of modes in a device ok.

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Modes – In summary

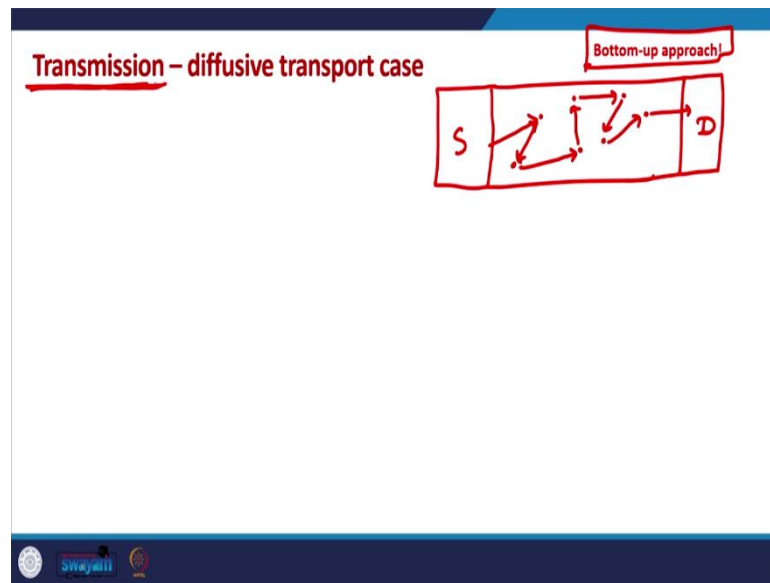
- The density-of-states vs. E is used to compute carrier densities.
- The number of modes (channels) vs. E is used to compute the current.
- The number of modes at energy, E , is proportional to the average velocity (in the direction of transport) at energy, E , times the density-of-states, $D(E)$.
- $M(E)$ depends on the band structure and on dimensionality.

The figure contains six subplots arranged in a 3x2 grid. The left column shows the density of states $D(E)$ and the right column shows the number of modes $M(E)$ as a function of energy E . The energy axis for all plots starts at E_c .

- 1D (top row):** D_{1D} is a step function that jumps at E_c and remains constant. M_{1D} is a step function that jumps at E_c and remains constant.
- 2D (middle row):** D_{2D} is a step function that jumps at E_c and remains constant. M_{2D} is a linear function starting from E_c .
- 3D (bottom row):** D_{3D} is a linear function starting from E_c . M_{3D} is a quadratic function starting from E_c .

So, that is all about the ballistic transport in a, the idea of modes in a ballistic transport case. Now, let us see how things turn out to be in the diffusive transport case .

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So, what is diffusive transport? If you recall from our earlier discussion, the diffusive transport is I would say more familiar way in which electrons transport. And in diffusive transport case if we have a 2 terminal device like this diffusive transport case is the case when the channel is long as compared to the to the mean free path of the electron. Mean free path is the distance or the mean distance average distance travelled by electron between 2 consecutive collisions.

And if the channel is very long as compared to this mean free path the distance between the 2 collisions, then there would be many collisions while electron is travelling from the source side to the drain side.

So, one of the ways in which the electrons motion can be visualized is this electron starts from the source it goes to a certain point it collides with maybe an atom there, it is reflected back possibly. Then here again it collides with somebody else, it may be goes straight again here it again reflects it collides maybe it goes up.

So, there is a constant or there is a continuous change of momentum while the electron is travelling here again a collision may come back or at a angle collides again maybe travels that side some of those electrons.

Some of these electrons they never reach from the source to the drain, some of the electrons that start from the source try to go to the drain they never reach there because of the

collisions. Some electrons reach there after multiple collisions, may be one of the possibilities could be like this ok.

So, this kind of transport is known as the diffusive transport and this kind of transport is there in our bulk devices as well and also the model or the way we conventionally understand conductivity and the transport of electrons is this kind of transport. Essentially the Drude's model was based on this assumption that electrons are colliding with intermediate hurdles, intermediate atoms or other things, vacancies may be and then they are going from the source to the drain side ok.

So, here the Drude's model or the classical theory of conduction that starts with this assumption, that this is the way the electrons are transporting and then they take the average of the motion in various directions. Here we will have a sort of bottom up approach, we now know how the electron transport in ballistic case when it directly goes from one terminal to another.

Now, building on top of that we will see how electrons behave when the transport is diffusive in nature, when the transport is not ballistic ok. So, this is a sort of bottom up approach of transport. We have first had a basic understanding of the ballistic transport now we are trying to see how a diffusive transport case will look like.

And there is this new term that comes in picture this is known as the transmission or transmission coefficient. A new idea of transmission coefficient comes into the picture in this case and that is what we will see.

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Transmission – diffusive transport case

Situation: A 2D electronic device with channel width, W and length, L .

Diffusive transport is assumed — the channel is many mean-free-paths long.

Now, in addition of the horizontal motion, vertical motion also happens.

Bottom-up approach!

$L \gg \lambda$
mean free path

So, just to sort of quickly sum it up for the sake of better visualization we take a 2D channel length and width in the channel electron is starting from the source side it is colliding with maybe many other things in the channel having a zigzag motion, all the electrons that start from the source may not reach the drain. In fact, they do not reach the drain because electron lose momentum.

It may also lose energy in between and it may not have sufficient energy to be, I would say attracted or pulled by the drain terminal and the channel is very long, the L is extremely large as compared to the mean free path where this parameter λ is the mean free path.

Please do not confuse this with λ_B which we discussed shortly before this discussion, λ_B is the de Broglie wavelength it is entirely different concept, here it is the wavelength in case of λ_B but this λ is the mean free path, it is the average distance travelled by electron while between 2 of its consecutive collisions ok.

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Transmission – diffusive transport case

Bottom-up approach!

Situation: A 2D electronic device with channel width, W and length, L .

Diffusive transport is assumed – the channel is many mean-free-paths long.

Electron undergoes a random walk from contact 1 to contact 2.

Now, in addition of the horizontal motion, vertical motion also happens.

Important quantity in conduction is: $\gamma \pi D / 2$

$$I = \frac{2e}{h} \int (\gamma \pi \cdot \frac{D}{2}) (f_1 - f_2) dE$$

So, now there is an interesting observation that we need to make here, we have the device like this long device now. The source side let us go back to the energy level scheme in the source side we have E_{Fs} , on the drain side we have E_{Fd} the Fermi level. In between the channel is very long, generally in long channels the discrete energy levels are not there.

There is a continuous electronic states maybe all these states are allowed. So, all these this is a continuum of states and all these states are allowed, maybe there is a band gap just above. So, just above we have a band gap and again there is a allowed range of energy values. Similarly, there could be a band gap here as well and all the electronic states below this state may also be allowed this is a band gap this is also a band gap and in between we have a continuum of energy states.

So, now this source side is trying to pump lot of electrons, it is trying to bring the channel in equilibrium with the left contact with the source contact. So, now, every electron that is injected from the source into the channel like this, it does not go straight away to the drain terminal. This does not happen in this case this was happening in the case of ballistic transport and that is why there we had the electron directly going from this point to this point.

And then on the drain contact the electron was losing energy up to the point of the drain Fermi level ok. In this case however, situation is different and electron is now starting maybe from this point to this point, it is colliding with intermediate maybe atoms sitting in the channel. Now, it might happen that this electron may lose energy and it go it might

go down, in the channel itself this energy may get dissipated in the collisions ok, that might actually make energy of some of the electrons.

So, for example, in this case this electron strikes with somebody here, loses some energy, it again goes in this direction maybe strikes again, loses some more energy go again loses some more energy here, it has come here. Now, this electron will not be taken by the drain terminal ok because the drain terminal is trying to bring the electrons up to its Fermi level the electronic population in the channel up to its Fermi level.

So, all the electrons that have energy above the drain Fermi level are taken by the drain contact. So, this electron may just end up in the channel somewhere may be losing energy or. So, all the electrons that start from the source side do not reach to the drain side and that is why in addition to the horizontal motion of electrons on the energy levels there is also a vertical motion happening in the diffusive transport case.

So, situation might be something like this, this is not exactly what is happening exact treatment comes from quantum mechanics, this is just a classical way of seeing things seeing how things are happening ok.

Now, with these conditions we can in other words say that now electrons undergo a random walk from contact 1 to contact 2 and as we have seen is that the important, one of the most important quantity in conduction is this.

So, if you recall in our derivation of current expression, we did not assume the nature of the transport. It was true both for ballistic transport or diffusive transport. So, the this expression of the current $\frac{2q}{h} \int \frac{\gamma(E)\pi D(E)}{2} (f_1 - f_2) dE$, this is true in general case, this is true in the case of ballistic transport, this is even true in the case of diffusive transport.

So, the important quantity is this and we have calculated this quantity in the case of ballistic transport. Now, we need to see what this quantity is in the case of diffusive transport ok.

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Transmission – diffusive transport case Bottom-up approach!

Situation: A 2D electronic device with channel width, W and length, L .

Diffusive transport is assumed – the channel is many mean-free-paths long.

Electron undergoes a random walk from contact 1 to contact 2.

Now, in addition of the horizontal motion, vertical motion also happens.

Important quantity in conduction is: $\gamma \approx D/l^2$

$M_D(E) = T(E) \cdot M_B(E)$

$T(E) \leq 1$

$\tau_D(E) \geq \tau_B(E)$

$\gamma_D(E) \leq \gamma_B(E)$

$M_D(E) \leq M_B(E)$

So, as anybody can guess that the transmission time, the characteristics time, the τ_E time in the case of diffusive transport this $\tau_D(E)$ will definitely be smaller than the ballistic transport case. In ballistic transport case, the electron is directly going from the source side to the drain side.

No collision channel is small, electron is directly in a single pathway electron is traveling through the channel. So, the transit time in the case of ballistic transport would definitely be sorry, will be smaller. So, the transit time in the case of diffusive transport will be larger as compared to the ballistic transport case. And in best case scenario when even in diffusive transport case there is no collision, it will be equal to the ballistic transport transit time.

So, if τ_D is the transit time in the case of diffusive transport, this will be larger than equal to τ_B . So, which means that gamma in the case of diffusive transport will be smaller than gamma in the case of ballistic transport, this energy broadening and this means this number of modes in diffusive transport case will be smaller than the number of modes in the ballistic transport case.

If M_D is the number of modes in diffusive transport case, it will be less than equal to the number of modes in the diffusive ballistic transport case. Let me write it here that now $M_D(E)$ can be written as $T(E)$ times $M_B(E)$ where $M_B(E)$ is the number of modes in the ballistic transport case and $M(E)$ is now in the diffusive transport case.

And this parameter $T(E)$ is known as the transmission coefficient and the value of $T(E)$ is always less than equal to 1. So, this is what we can easily say just by looking at the situation that is there in the case of diffusive transport case.

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Transmission – diffusive transport case

Bottom-up approach!

Situation: A 2D electronic device with channel width, W and length, L .

Diffusive transport is assumed — the channel is many mean-free-paths long.

Electron undergoes a random walk from contact 1 to contact 2.

Now, in addition of the horizontal motion, vertical motion also happens.

Important quantity in conduction is: $\gamma\pi D/2 = M(E) \cdot T(E)$

In diffusive transport case: $\gamma\pi D/2 = M(E)T(E)$. $T(E) \leq 1$

Where: $T(E) \leq 1$ Transmission.

It is nothing, I would say or this quantity can now be written as number of modes times $T(E)$, where $T(E)$ is less than equal to 1. Actually the number of modes would not change in the device.

So, saying that number of modes in diffusive transport case is not a physically accurate idea. So, that was just to sort of convey the message that this quantity will now be smaller than the quantity that was there in the case of ballistic transport case and this is known as the transmission coefficient.

So, in our next class, we will describe or we will analyze the transmission coefficient and we will analyze this quantity $\frac{\gamma\pi D}{2}$ in better details more mathematically. So, until then I would recommend you to again go back to the to the derivation of modes in ballistic transport case and that would be definitely helpful in understanding our forthcoming analysis. So, that is all for this class.

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