Physics of Nanoscale Devices
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Lecture - 60
Quantum Dot Devices – IV Characteristics, DFT Course Summary

Hello everyone and welcome to this welcome to this concluding class of this course and as you might be aware that in this class we will discuss the Quantum Dot Devices, specifically we will discuss the IV Characteristics of the devices of these devices.

And then we will have a short and I would say introductory discussion on the density functional theory which is an ab intio way of doing of calculating the electronic structure of nanosystems. And then we will briefly have we will briefly go through the entire course or we will have an overview of the course summary.

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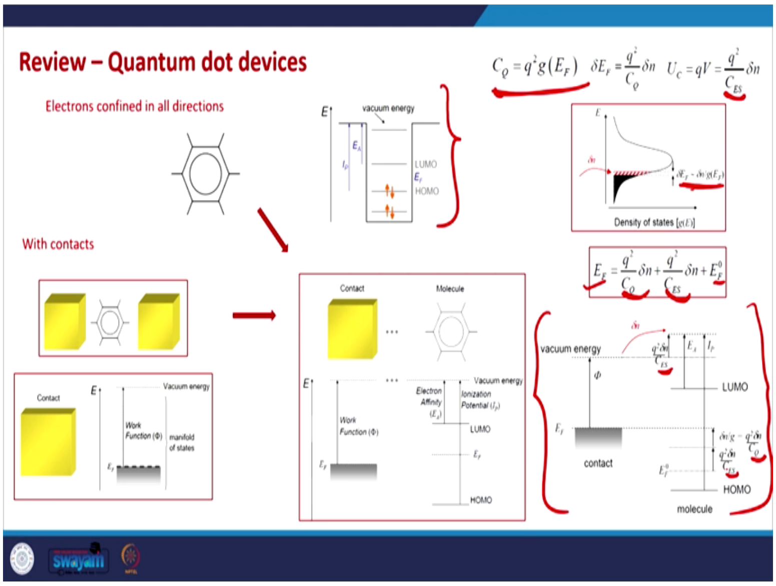

Review – Quantum dot devices

Electrons confined in all directions

With contacts

$C_Q = q^2 g(E_F)$ $\delta E_F = \frac{q^2}{C_Q}\delta n$ $U_C = qV = \frac{q^2}{C_{ES}}\delta n$

$E_F = \frac{q^2}{C_Q}\delta n + \frac{q^2}{C_{ES}}\delta n + E_F^0$

So, let us quickly review what we have been discussing. So, what we have seen. So, far is that in quantum dot devices the device the channel part the active part of the device that is modeled in this way by using molecular orbital’s.

And we have seen what happens when we put this quantum dot in contact with metallic bulk metal. So, when the contacts are of bulk metal and we have a quantum dot in between then in equilibrium the change in the Fermi level happens. Because of the two processes one is the quantum capacitance and second is because of the electrostatic effect.

So, when there is a there is a change in the number of electrons on the quantum dot just because of the change in the number the Fermi level might change and this is accounted for by the quantum capacitance. Similarly when there is a change in the number of electrons on the system that also changes the charge on the system that changes the electrostatic potential energy of the system and that is accounted for by the electrostatic capacitance of the device.

And in total we need to consider both of these effects and. So, that is why the Fermi level of the device can be written as the Fermi level of the quantum dot without any connection without the contacts plus the contribution in the change of Fermi level due to quantum capacitance and the contribution due to the electrostatic capacitance.

And pictorially this is represented in this way as you can see here. So, the key point here is that the change in the vacuum energy is just because of the electrostatic capacitance, but the change in the Fermi level is because both the quantum capacitance and the electrostatic capacitance. So, that is the key thing that we need to keep in mind while understanding the quantum dot devices.

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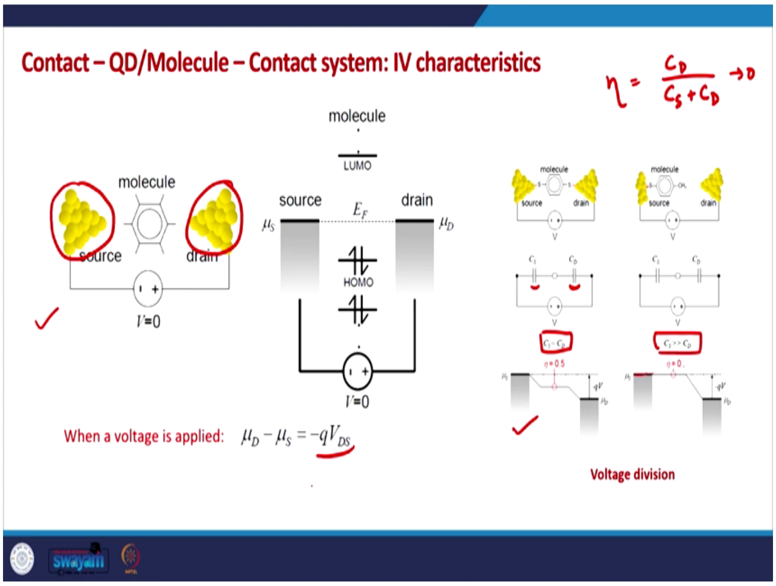

Contact – QD/Molecule – Contact system: IV characteristics

$\eta = \frac{C_D}{C_S + C_D} \to 0$

When a voltage is applied: $\mu_D - \mu_S = -qV_{DS}$

Voltage division

Then if we put a quantum dot and we put two contacts bulk contacts on this quantum dot. This is the kind of device that we obtain and these are the connections of the bulk contacts to the molecule or the quantum dots. And when there is no bias in that case the Fermi level across this entire device is uniform the Fermi level of the source the drain and the molecule are at the same level.

When we apply a voltage as we also discussed in the last class we need to understand two things here one is how is the voltage divided across the or how does the voltage drop across the device. In other words where does the voltage drop in this device and that depends on the these two capacitors. The source and the drain capacitors which essentially models the interface between the source and the molecule and the source and the drain and the molecule.

So, if both of these capacitors both of these interface capacitors are same in that case the voltage drops equally at both the interfaces in this way. And if one of the capacitances is large let us say if the molecule is closer to the source contact as compared to the drain contact.

In that case this voltage division factor which we defined in the previous class which is given as $C_D/(C_S + C_D)$ this tends to 0 and in that case almost the entire voltage drops across the molecule drain interface and not across the source and the molecule interface.

So, accordingly we can understand the electron transfer in this in these devices. The second thing that we need to understand is in when there is an applied voltage when drain voltage is applied it means that now the equilibrium is disturbed. So, in this case there will be there might be an electron transfer through this device which will change the number of electrons in the molecule which will change the potential energy of the system as well.

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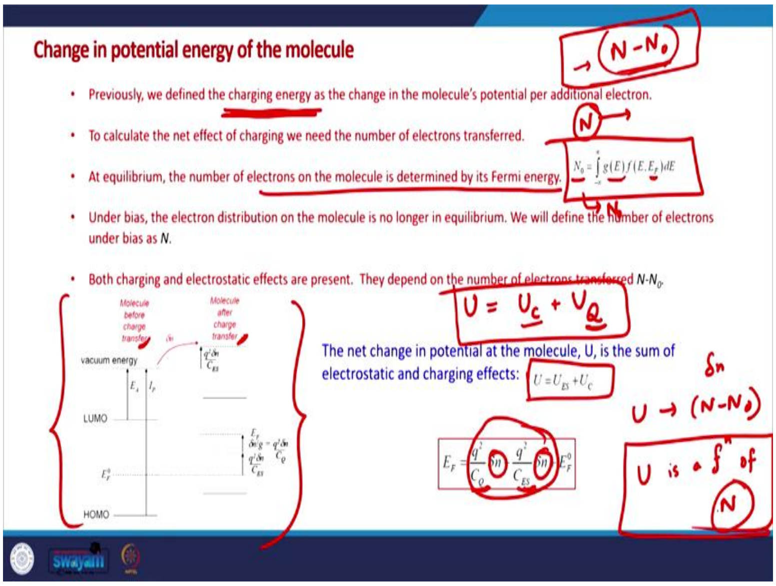

Change in potential energy of the molecule

- Previously, we defined the charging energy as the change in the molecule's potential per additional electron.
- To calculate the net effect of charging we need the number of electrons transferred.
- At equilibrium, the number of electrons on the molecule is determined by its Fermi energy. $N_0 = \int_{-\infty}^{\infty} g(E) f(E, E_F) dE$
- Under bias, the electron distribution on the molecule is no longer in equilibrium. We will define the number of electrons under bias as N.
- Both charging and electrostatic effects are present. They depend on the number of electrons transferred N-N_0.

The net change in potential at the molecule, U, is the sum of electrostatic and charging effects: $U = U_{ES} + U_C$

$E_F = \frac{q^2}{C_Q}\delta n + \frac{q^2}{C_{ES}}\delta n + E_F^0$

$\rightarrow (N - N_0)$

$N \rightarrow$

$\hookrightarrow N$

$U = U_C + U_Q$

δn

$U \rightarrow (N - N_0)$

U is a f^n of N

So, this change we need to understand because the density of states depends on this the potential energy of the system ok. So, as we discussed in the previous class the change in the potential energy is because of the two components. One is because of the charging energy which is the electrostatic component and second is the because of the state filing which is because of the change in the number of electrons on the system.

So, if at equilibrium if the number of electrons on the molecule were N_0, which is governed by the equilibrium Fermi level of the system E_F and the density of states of the system. So, this is the equilibrium number of electrons on the quantum dot or on the molecule, but now this equilibrium is disturbed and very soon steady state will be established.

Steady state by definition is the state when the current through the device is constant ok. So, in this case the number of electrons in steady state might be different than the equilibrium number of states during this discussion. I would recommend all of you to please have the discussion on the general model of transport in the back of your minds.

Because in that way you can draw parallels between the two and this will also become easier to understand. So, in steady state if the number of electrons in the molecule is N in equilibrium the number of electrons on the molecule or on the quantum dot is N_0. So, there is this net change of $N - N_0$ on the quantum dot.

And this change in the number of electrons will change the potential energy in two ways. One is the charging energy, second is the state filling energy. Charging energy is modeled by the electrostatic capacitance and the state filling is modeled by the quantum capacitance.

So, that way this is the picture of the electronic energy levels both before the charge transfer and after the charge transfer. So, the net charge transfer is N - N_0 on the quantum dots. So, this will bring a change in the potential energy which is a sum of charging energy plus the energy because of the state filling.

The charging energy is modeled by the electrostatic capacitance and the state filling is modeled by the quantum capacitance. So, this discussion we have had now multiple times. So, finally, the total I would say the total change in the potential energy can be written as a sum of these two components.

And these two components are essentially written here and this will there is a key point here. This U, the change in the potential energy of the system depends on the number of electrons transferred because it depends on δN and δN is N - N_0.

So, U is a function of N here, N is the steady state number of electrons on the quantum dot when a drain voltage is applied when there is a bias across the quantum dot device. Please keep this in mind that the potential energy of the quantum dot is a function of the steady state number of electrons on the quantum dot.

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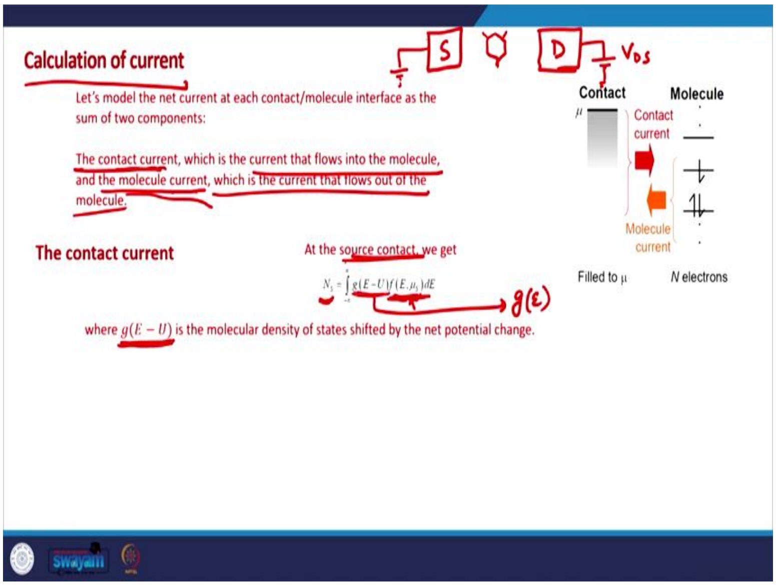

Calculation of current

Let's model the net current at each contact/molecule interface as the sum of two components:

The contact current, which is the current that flows into the molecule, and the molecule current, which is the current that flows out of the molecule.

The contact current

At the source contact, we get

$$N_S = \int_{-\infty}^{\infty} g(E-U) f(E,\mu_S)\, dE$$

where $g(E-U)$ is the molecular density of states shifted by the net potential change.

Now, with this we are in a position to sort of calculate the current across this system. So, the system that we have is the source contact, the drain contact and a molecular quantum dot in a way in order to properly understand the current flow in this device when we apply a positive voltage on the drain contact when a V_{DS} is applied.

Let us break the to the current in the steady state in two components. One is known as the contact current which is the current that flows into the molecule. The current from the contacts to the molecule is termed as the contact current and the second component of the current is the molecule current which is the current that flows out of the molecule.

The total current will be a sum of proper sum of these two components ok. So, the reason that we are dividing the current in the system in two components the contact current and the molecule current is that the contact current depends on the occupancy of energy levels in the contacts it depends on the number of electrons in the contacts.

And the molecule current depends on the number of electrons in the molecules ok. So, that is why we have divided these two the total current in these two components. So, the contact current depends on the Fermi functions of the contacts. So, the source contact current which is the current that flows into the molecule from the source is given by or is will depend on the number of electrons going from the source to the molecule.

So, what the source tries to do is the source tries to fill the quantum dot up to the source Fermi level or in other words the source tries to fill the states in the quantum dot according to the Fermi function of the source ok. So, these are the number of electrons that the source can pump into the molecule or into the quantum dot.

This is given by the density of states of the molecule times the Fermi function of the source. Please if we if you recall the general model of transport in that case also we had a similar term while calculating the rate of flow of electrons from the source into the molecule there is a key point here.

This density of state is the molecular density of state and this is now shifted by the change in the potential in the molecule that is brought about by the change in the number of electrons in our previous discussion in the general model of transport this g(E) did not had U in the argument. So, the density of states here in this expression was just g(E), but now we need to have g(E-U) ok.

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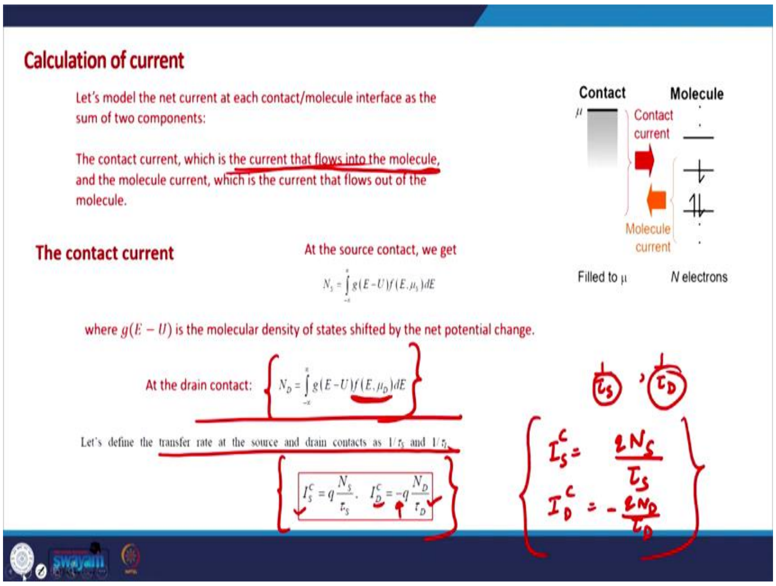

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where $g(E-U)$ is the molecular density of states shifted by the net potential change.

At the drain contact: $N_D = \int_{-\infty}^{\infty} g(E-U) f(E,\mu_D)\, dE$

Let's define the transfer rate at the source and drain contacts as $1/\tau_S$ and $1/\tau_D$

$$I_S^C = q\frac{N_S}{\tau_S}, \quad I_D^C = -q\frac{N_D}{\tau_D}$$

τ_S , τ_D

$$I_S^C = \frac{qN_S}{\tau_S}$$

$$I_D^C = -\frac{qN_D}{\tau_D}$$

So, similarly at the drain contact, the drain tries to would try to fill the quantum dot according to the Fermi distribution of the drain or it will try to fill all the electronic states up to the drain Fermi level. So, the number of electrons available at the drain for current conduction is given by this number.

So, if we define the rate transfer rate at the source and the drain contacts are as $1/\tau_S$ and $1/\tau_D$, τ_S and τ_D can also be termed as the transit times from the source contact and the drain contacts. So, with this the contact current which is just because the current component because of the electrons in the contacts is given by the source contact current is given as q times N_S divided by τ_S and the drain contact current is given as -q times N_D divided by τ_D.

Generally the reason for this negative sign is generally what happens is a positive voltage on the drain side allows electrons from the source to go into the molecule and from molecule to the drain.

So, that is why this negative sign is there this we have taken a convention if the electrons are going from the contact into the molecule the current is defined as positive and if the electrons are going from the molecule to the contact it is defined as negative.

So, this is just the contact component of the current, which so the current is given as the charge transfer which is q times N_S divided by the rate time that it takes for the charge to travel through the device. Similarly so this is the source contact current similarly the drain contact current will be q times N_D divided by τ_D and minus because electrons are going from the molecule to the drain. So, this is just the contact component of the current.

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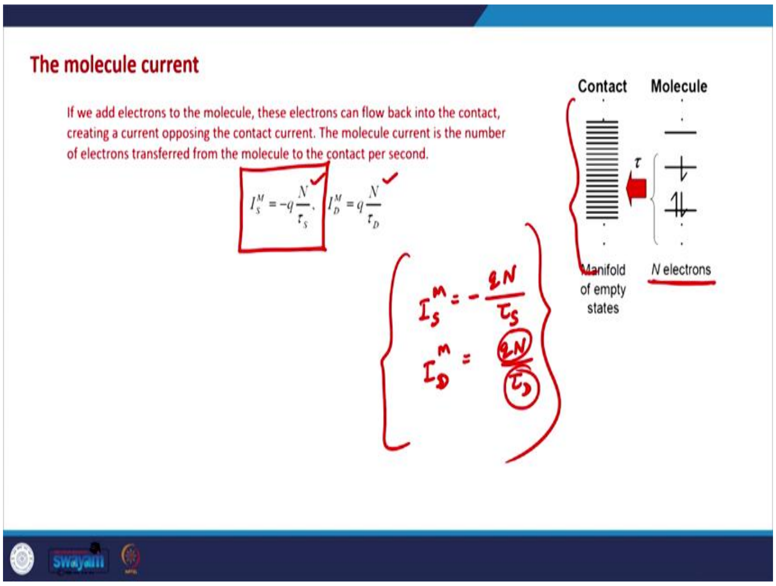

The molecule current

If we add electrons to the molecule, these electrons can flow back into the contact, creating a current opposing the contact current. The molecule current is the number of electrons transferred from the molecule to the contact per second.

$$\boxed{I_S^M = -q\frac{N}{\tau_S}},\ I_D^M = q\frac{N}{\tau_D}$$

$$I_S^M = -\frac{qN}{\tau_S}$$

$$I_D^M = \frac{qN}{\tau_D}$$

Now, let us come to the molecule current. So, the molecule might have will have N number of electrons in the steady state and what happens is if these electrons see any empty state in the contact then these electrons can hop from the molecule to the contact. The contacts as all of us know by now that the contacts are the continuum states the contacts have continuum of states .

So, there might be some empty states as well because of the if we go by the Fermi distribution function at finite temperature there might be empty states corresponding to the filled energy levels in the molecule. So, there might be a component of current that is because of the electron transfer from the molecule to the contact ok.

So, this is given as this is termed as the molecule current and this depends on the number of electrons in the molecule as similar to the because the contact current depends on the number of electrons in the contacts, number of electrons available in the contacts for the conduction.

Similarly the number of electrons in steady state in the molecule is N and if they find any empty state either in the source or in the drain side they can hop into those states and that will contribute in the molecular current.

So, the molecular current on the source side is the charge in the molecule divided by the time that it takes for discharge to go to the contacts and in steady state for positive drain voltage generally the electron flow is from source to molecule to the drain. So, that is why this is there is a negative sign here.

Similarly, the molecule current in the drain contact is the charge available in the molecule divided by the time that it takes for discharge to transit to the drain side ok. So, these are the molecular components in the previous slide we have the contact components.

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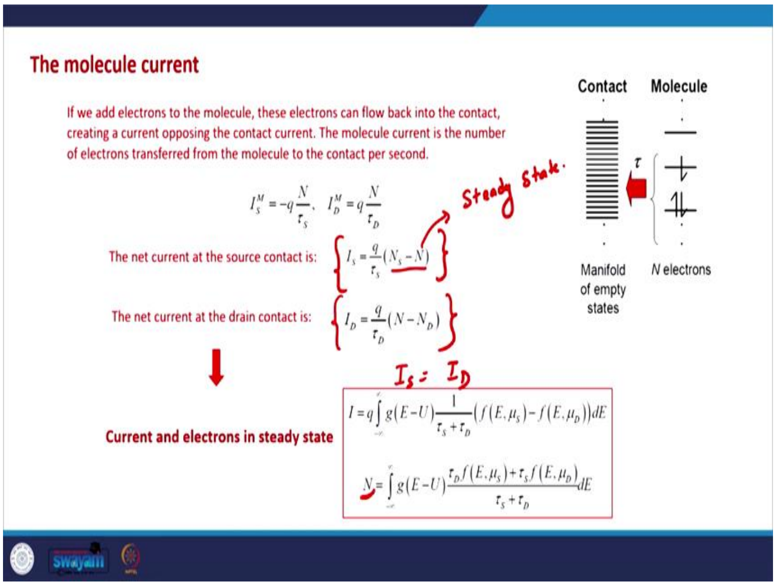

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If we add electrons to the molecule, these electrons can flow back into the contact, creating a current opposing the contact current. The molecule current is the number of electrons transferred from the molecule to the contact per second.

$$I_S^M = -q\frac{N}{\tau_S}, \quad I_D^M = q\frac{N}{\tau_D}$$

The net current at the source contact is: $\left\{ I_S = \frac{q}{\tau_S}\left(\underline{N_S - N}\right) \right\} \nearrow$ Steady State.

The net current at the drain contact is: $\left\{ I_D = \frac{q}{\tau_D}\left(N - N_D\right) \right\}$

↓

$I_S = I_D$

Current and electrons in steady state

$$\boxed{\begin{aligned} I &= q\int_{-\infty}^{\infty} g(E-U)\frac{1}{\tau_S+\tau_D}\left(f(E,\mu_S) - f(E,\mu_D)\right)dE \\ N &= \int_{-\infty}^{\infty} g(E-U)\frac{\tau_D f(E,\mu_S) + \tau_S f(E,\mu_D)}{\tau_S+\tau_D}dE \end{aligned}}$$

So, finally, the net current in these systems is the sum of these two components. So, the source component of the current is (q/τ_S) $(N_S - N)$. And similarly the drain component is (q/τ_D) $(N - N_D)$; where N is the number of electrons in the quantum dot in steady state and N_S and N_D are the number of electrons in the source and the drain contacts.

And if we in steady state these two there is a constant current through the throughout the device. So, this I_S should be equal to I_D and if we equate these two expressions and if we replace it back to these expressions as well. Then we obtain the expressions for the steady state electrons in the quantum dot and the steady state current in the system.

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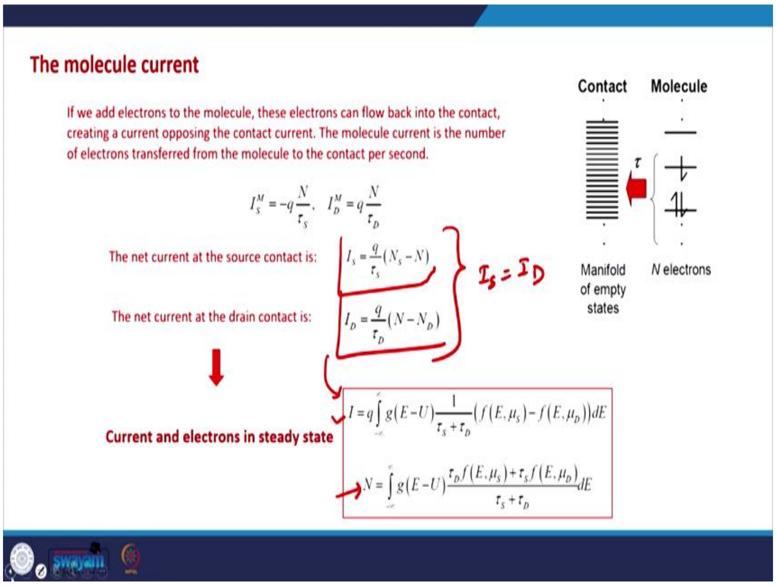

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The net current at the source contact is: $I_S = \frac{q}{\tau_S}(N_S - N)$

The net current at the drain contact is: $I_D = \frac{q}{\tau_D}(N - N_D)$

$I_S = I_D$

Current and electrons in steady state

$$\boxed{\begin{aligned} I &= q\int_{-\infty}^{\infty} g(E-U)\frac{1}{\tau_S+\tau_D}\left(f(E,\mu_S)-f(E,\mu_D)\right)dE \\ N &= \int_{-\infty}^{\infty} g(E-U)\frac{\tau_D f(E,\mu_S)+\tau_S f(E,\mu_D)}{\tau_S+\tau_D}dE \end{aligned}}$$

By equating these two equations by putting them equal to each other. Because in steady state I_S is equal to I_D we will obtain the expression for N and if we replace this N into this equation or this equation we will obtain an expression for I. So, I would recommend all of you to do this derivation. So, I am skipping this step and as I said this is quite similar to the to the calculation that we did in the general model of transport.

It is it has it actually draws parallels from there N_S and N_D are given by the expressions in the previous slides these expressions essentially ok depends on the source Fermi distribution and the drain Fermi distribution function. So, with this we have the expressions for the steady state electronic number and the steady state current in the device ok.

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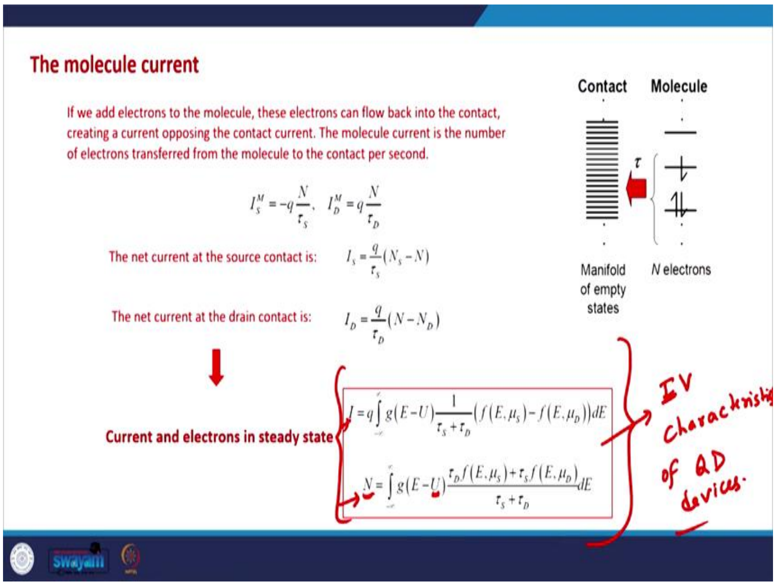

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Current and electrons in steady state

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IV characteristi
of QD
devices.

So, this is the IV characteristics now this gives the IV characteristics of the quantum dot device on any nanostructure in a way ok. But if you have a careful look at these equations there is a catch in these equations and the catch is that N which is the number of electrons it depends on U, because the density of states depends on U.

And U in turn depends on N because if you go back and just to quickly review the change in potential U is a function of N it depends on N it. In fact, U depends on δN which is N - N_0, N_0 is the equilibrium number of electrons.

So, that is the catch in these equations that the steady state number of electrons depend on U which is in turn function of N. So, this is not a closed form solution or this is not a closed form equation I would say we cannot have a closed form solution of these equations.

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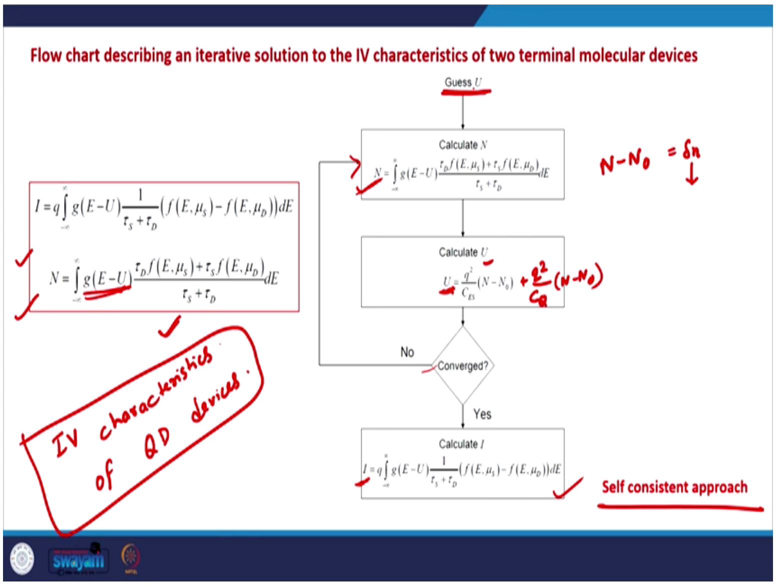

Flow chart describing an iterative solution to the IV characteristics of two terminal molecular devices

$$I = q\int_{-\infty}^{\infty} g(E-U)\frac{1}{\tau_S+\tau_D}\left(f(E,\mu_S)-f(E,\mu_D)\right)dE$$

$$N = \int_{-\infty}^{\infty} g(E-U)\frac{\tau_D f(E,\mu_S)+\tau_S f(E,\mu_D)}{\tau_S+\tau_D}dE$$

IV characteristics of QD devices.

Guess U

Calculate N

$$N = \int_{-\infty}^{\infty} g(E-U)\frac{\tau_D f(E,\mu_S)+\tau_S f(E,\mu_D)}{\tau_S+\tau_D}dE$$

$$N-N_0 = \delta n$$

Calculate U

$$U = \frac{q^2}{C_{ES}}(N-N_0) + \frac{q^2}{C_Q}(N-N_0)$$

Converged?

No

Yes

Calculate I

$$I = q\int_{-\infty}^{\infty} g(E-U)\frac{1}{\tau_S+\tau_D}\left(f(E,\mu_S)-f(E,\mu_D)\right)dE$$

Self consistent approach

And that is why what we do is with these equations we need to do the what is known as the we need to in order to solve these equations. We need to use the iterative method or what is known as the self consistent solution self consistent approach to solve these equations.

So, the way this works is that we make an initial guess of U and with this guess we calculate the density of states and calculate the steady state number of electrons in the system from this value. From this N we can calculate N - N_0 which is δN and from δN we further calculate U, which is this and this will also have the quantum capacitance component ok.

Then with this U this new U that we obtain in this step we compare this with our initial guess and if both of them match with fair accuracy they are fairly close to each other or they converge to a particular value. Then we take that to be the final U and based on that U, we calculate the steady state current in the system.

But if this and the initial guess do not match then we again go back to this step. We again with this U we calculate N from this N we calculate a new U we compare this one and the previous one. If they converge then we calculate the steady state current otherwise we go back. So, this is the iterative way to calculate the solution of these equations.

Because we cannot have the closed form solution and this is known as the self consistent approach to solve these equations and this essentially completes our calculations of calculation of IV characteristics of the quantum dot devices ok. So, I would all again recommend you to go back and derive these two equations from the contact current and the molecule current.

And then this iterative or the self consistent approach will give us the final solution of the steady state current and the steady state number of electrons in the system ok. So, that is essentially what we have on the quantum dot devices, two terminal quantum dot devices and this discussion can also be extended to the three terminal devices. The way we extended the general model of transport discussion to MOSFET transfer as well ok.

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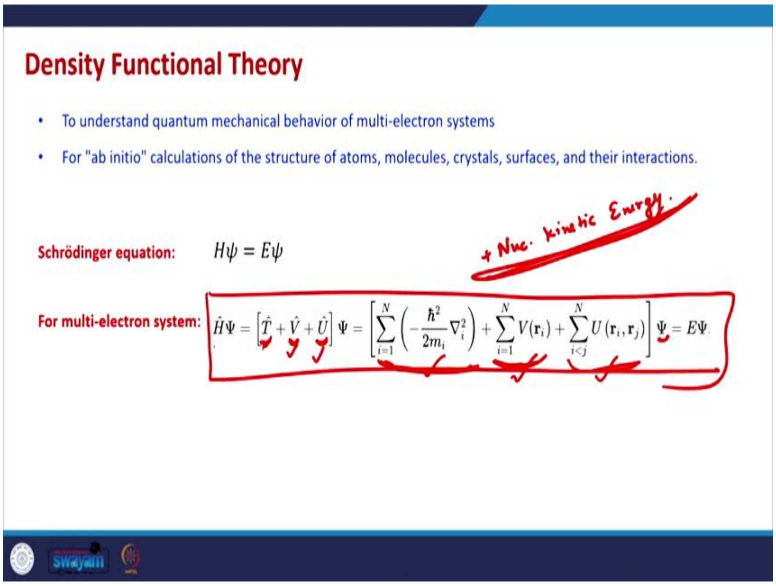

Density Functional Theory

- To understand quantum mechanical behavior of multi-electron systems
- For "ab initio" calculations of the structure of atoms, molecules, crystals, surfaces, and their interactions.

Schrödinger equation: $H\psi = E\psi$

+ Nuc. kinetic Energy.

For multi-electron system: $$\hat{H}\Psi = \left[\hat{T}+\hat{V}+\hat{U}\right]\Psi = \left[\sum_{i=1}^{N}\left(-\frac{\hbar^2}{2m_i}\nabla_i^2\right)+\sum_{i=1}^{N}V(\mathbf{r}_i)+\sum_{i<j}^{N}U(\mathbf{r}_i,\mathbf{r}_j)\right]\Psi = E\Psi$$

So, with this now we come to our last topic of this course which is the density functional theory. So, it has prominently it has two terms, one is the density, second is the functional. So, this is the theory or this is a method to understand the quantum mechanical behavior of many body systems, multielectron systems, nanosystems actually and this is an ab intio approach ab intio method to calculate the electronic structure of atoms molecules crystals surface and their interaction.

So, it is heavily used in computational chemistry it is used in condense matter physics, it is used in electronics it is used in material science nowadays. So, this is one of the I would say most important quantum mechanical method to understand the electronic structure electronic properties and also nowadays magnetic properties of the atoms from first principles.

Because in our discussion of in our previous discussion what we have assumed is that we know what is the band structure of the device. What is the band structure of the channel and from that we can calculate the density of states from that we can from there we can calculate the modes we can calculate the current.

We can calculate almost all the electronic properties electronic characteristics of the device. But if we have a novel structure if we have a new kind of structure where we do not know anything we do not know about it is Ek relationship. We do not know about it is about it is band structure we need to start from the first principles.

And that is why it is known as the ab initio method it makes some approximations because without approximations we cannot solve the quantum mechanical equations and very soon it will be clear why this is known as the density functional theory ok. So, let us begin with the basics of this if we have any quantum system all the information about that system is encapsulated in the wave function of that system.

And the wave function is obtained from the Schrodinger equation. The Schrodinger equation is a very simple I would say simple and elegant equation it relates the Hamiltonian which is the total energy operator of the system. And if we operate this Hamiltonian on the wave function of the system it will it gives us the energy corresponding to that wave function.

So, by solving this equation we can obtain the energy states various energy states and various eigen states and eigen values energy states as well as the wave functions corresponding to those states ok. So, this is where we need to start from if we try to understand any new system any unknown system.

This is the starting point, but for multielectron systems. For example, in a quantum dot system where we have few hundreds of atoms in which we have let us say few hundreds of electrons interacting with each other only external electrons are interacting let us say outer orbital electrons are interacting let us say. So, in multi electron systems the Schrodinger equation transforms into this way.

This Hamiltonian now has three components prominently three components one is the kinetic energy of the electrons which is given by the kinetic energy operator let say there are N number of electrons in the system, capital N number of electrons.

So, the Hamiltonian which is the total energy operator is essentially the sum of the total energy of the electrons will be the sum of kinetic energy plus the interaction energy of that arises. Because of the interaction of electrons with the nuclei in the system or atomic course in the system positively charged atomic course in the system that is given by this second term.

And third is this electron electron interaction which is given by this third term. So, this is the scenario in multielectron system there is in total energy there is this nuclear kinetic energy term as well. But since it is assumed that the nuclei various nuclei in a system are almost fixed because the mass of the nuclei nucleus is extremely large as compared to the mass of electrons.

So, their velocity is or their they do not basically move their kinetic energy is assumed to be negligible. And if we are only interested in the electronic structure these are the three components of electronic energy that we need to consider, one is the kinetic energy of electrons given by the kinetic energy operator.

Second is the electronic interaction with nuclei given by this electrostatic potential V third is the electron, electron interaction given by the electrostatic potential energy U. And if we in this N electron system if we try to find out all the properties of this system we are trying to understand the system.

We need to finally, calculate the wave function of this system. And we need to put this Hamiltonian in Schrodinger equation and this is finally, what we obtain this is the equation that we need to solve for N electron system.

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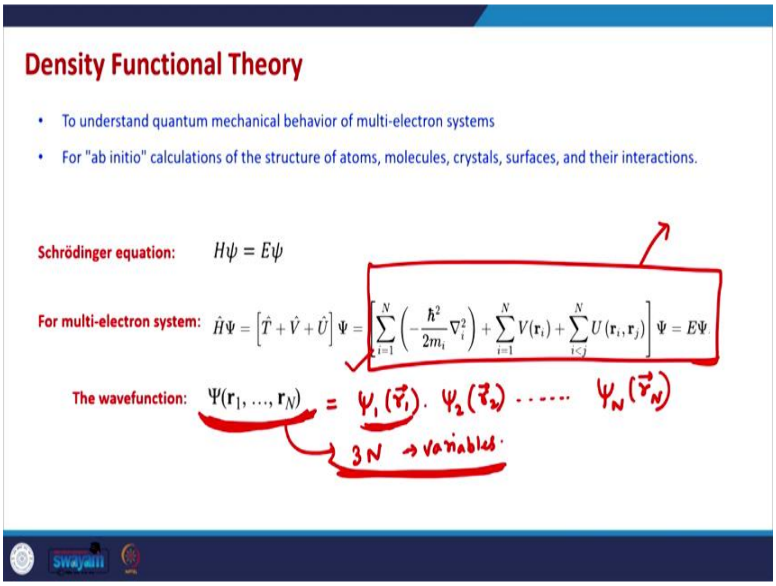

Density Functional Theory

- To understand quantum mechanical behavior of multi-electron systems
- For "ab initio" calculations of the structure of atoms, molecules, crystals, surfaces, and their interactions.

Schrödinger equation: $H\psi = E\psi$

For multi-electron system: $\hat{H}\Psi = \left[\hat{T} + \hat{V} + \hat{U}\right]\Psi = \boxed{\left[\sum_{i=1}^{N}\left(-\frac{\hbar^2}{2m_i}\nabla_i^2\right) + \sum_{i=1}^{N} V(\mathbf{r}_i) + \sum_{i<j}^{N} U(\mathbf{r}_i, \mathbf{r}_j)\right]\Psi = E\Psi}$

The wavefunction: $\underbrace{\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)}_{3N \rightarrow \text{variables}} = \underline{\psi_1}(\vec{r}_1) \cdot \psi_2(\vec{r}_2) \cdots\cdots \psi_N(\vec{r}_N)$

For a multielectron system the wave function looks like this which is essentially the product of the wave functions of different electrons. And if you have a careful look each of these wave function. So, this Ψ_1, Ψ_2, Ψ_N are the wave functions of first electron second electron and nth electron. And if we have a careful look each of these wave functions is this Ψ each of these Ψ is a function of three variables three space variables.

If we are just considering the space dimension we are not considering the time evolution at the moment and this N electron wave function is a function of 3N variables now and that is a problem actually. So, in multielectron systems, this Schrodinger equation involves a wave function that is a function of 3N variables.

And if N is few hundred atom few hundred electrons only few hundred electrons small systems even in that case this equation becomes almost impossible or impossible to solve. Actually this becomes unsolvable and that is the, in other words what we can say that is the curse of the dimensionality.

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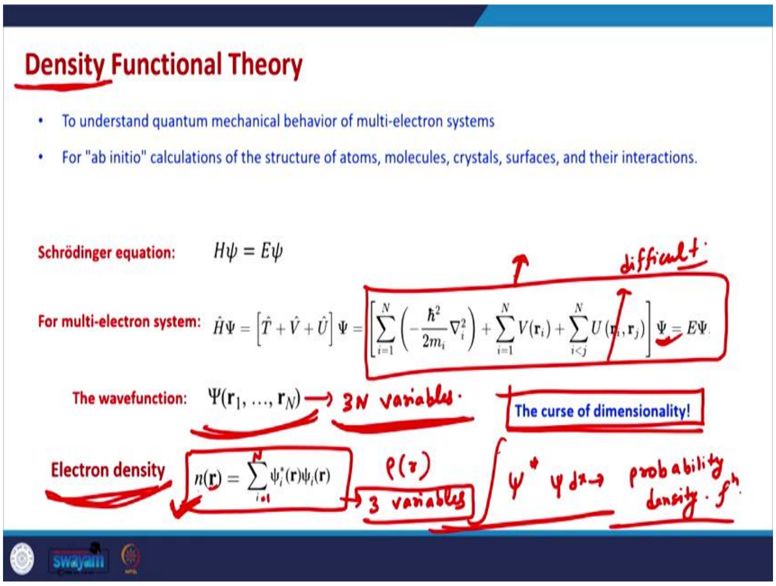

Density Functional Theory

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difficult.

The wavefunction: $\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \rightarrow$ 3N variables.

The curse of dimensionality!

Electron density $n(\mathbf{r}) = \sum_{i=1}^{N}\psi_i^*(\mathbf{r})\psi_i(\mathbf{r}) \rightarrow$ 3 variables

$\rho(r)$

$\int \psi^* \psi \, dx \rightarrow$ probability density. f^n.

Because as the number of electrons increase in a system the dimensionality the dimension of the wave function increases which increases the dimension. And the correspondingly the dimension of all the operators Hamiltonian will increase the calculation will become just impossible. So, we cannot directly solve the Schrodinger equation for this system one reason is this second is this.

This interaction is also extremely difficult this interaction. So, instead of dealing with the wave function what we deal with is the density of electrons which is defined as in this way I is from 1 to N, $\Psi_i^* \Psi_i$ summation of all the electrons. So, if you remember $\Psi^* \Psi$ is known as the probability density.

So, this gives us this is known as the probability density function and if we integrate this over space. This gives us the probability that an electron will be found in a certain region of the space from on the similar lines this electron density function is defined for all the electrons.

So, what we assume is? We assume as if there is an electron distribution in the system, N electrons are distributed in a certain way and this is defined by n or sometimes ρ as well. And now this probability or this electron density function is just a function of three space variables it is just a function of three variables whatever be the number of electrons whatever be capital N if you just to quickly remind the wave function is a function of 3N variables.

But the electron density is a function of just three variable three space variables. If we are considering the if we are just considering the time dependent part. If we can somehow sort of reformulate this Schrodinger equation, in terms of this electron density function. Then we would not need to deal with 3N variables in the wave function and large matrices.

And in that way we can somehow manage the this calculation and that is essentially that lies at the heart of the density function in theory that is where this first term density comes in this DFT. Because instead of directly dealing with the wave function of electrons it deals with the electron density function.

Whatever be the number of electrons the electron density function will just be a function of 3 variables. So, this curse of dimensionality has been will be or is dealt with by dealing with the electron density function instead of dealing with the electronic wave function, but how do we deal with this electron density function. How do we solve or in a way solve this Schrodinger equation using electron density function.

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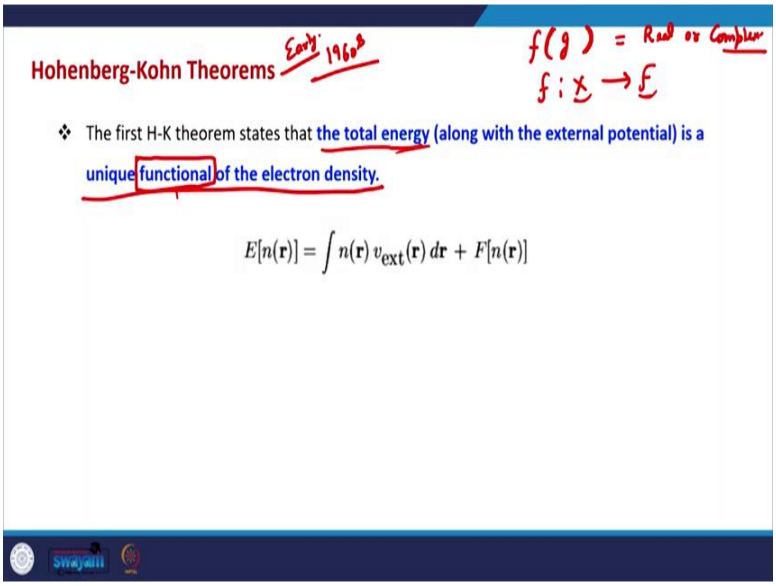

Hohenberg-Kohn Theorems Early 1960s

$f(g) = \text{Real or Complex}$

$f : X \rightarrow E$

- The first H-K theorem states that the total energy (along with the external potential) is a unique functional of the electron density.

$$E[n(\mathbf{r})] = \int n(\mathbf{r})\, v_{\text{ext}}(\mathbf{r})\, d\mathbf{r} + F[n(\mathbf{r})]$$

And the I would say this the credit goes to the two theorems given by Hohenberg and Kohn in early 1960s. So, what these theorems do? They sort of reformulate our problem of solving multi dimensional Schrodinger equation in solving or finding out the electron density. So, let us let us go through the theorems first and then it will become clear.

So, what the first H K theorem Hohenberg Kohn theorem says is that the total energy of the system is a unique functional of the electron density. So, what it means is? If we go back to the previous slide the electronic energy the energy of the system depends on the Hamiltonian according to the Schrodinger equation depends on the Hamiltonian.

And we need to solve the Schrodinger equation, but what H K theorem says is that this energy of the system is a unique functional of the electron density. So, we can somehow calculate the energy from the electron density it depends on just on the it is a unique function.

And now this functional is a new term here functional essentially is means the functional means functional is a function actually. So, it is a function whose argument is also another function ok. So, in a way very loosely define defining very loosely it is a function of functions more rigorously it is a function which maps from a space of functions to a field of scalar a field of real or complex numbers.

So, it is a map from the space of functions to the field of real or complex numbers in simple words the argument of a functional is a function and it gives us a real or complex number that is known as the function. So, what this first H K theorem says is that the total energy is a unique functional of the electron density.

And that is where this second term in this DFT comes from. So, it deals with electron density and it deals with the energy function because energy is a functional of the density which means the energy of the electrons is a function of electron density function ok. So, the first theorem reduced or first theorem sort of conveyed that the energy can be calculated from the just from the electron density function.

And this is sort of the form of this energy functional the energy functional can be written as sum of two components. One is because of the external potential; external means interaction of electrons with nuclei with atomic course plus in a way intrinsic energy functional.

We will come back to this is because of the electron electron interaction in the system primarily plus the kinetic energy. But kinetic energy is not dependent on the electron density. So, it depends on the electron electron interaction.

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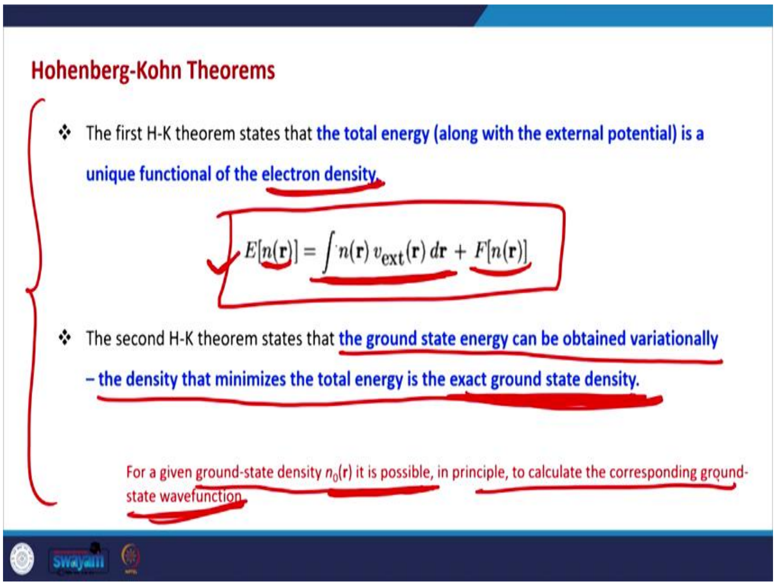

Hohenberg-Kohn Theorems

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$$E[n(\mathbf{r})] = \int n(\mathbf{r})\, v_{\text{ext}}(\mathbf{r})\, d\mathbf{r} + F[n(\mathbf{r})]$$

- The second H-K theorem states that **the ground state energy can be obtained variationally – the density that minimizes the total energy is the exact ground state density.**

For a given ground-state density $n_0(\mathbf{r})$ it is possible, in principle, to calculate the corresponding ground-state wavefunction.

The second theorem says what the second theorem says is second H K theorem that the ground state energy can be obtained variationally; variationally means by minimizing it as a function of the electron density. So, the electron density that minimizes the total energy is the ground state exactly the ground state density of the system.

So, what it says is that we need to find out the electron density function n r and we need to find out that electron density which minimizes the total energy function and that will be the ground state electron density function. And as a consequence or one of the consequences of this H K theorems is that or one of one of the I would say side results is that from a ground state density function from the ground state density of electrons.

In principle it is possible to calculate the corresponding ground state wave function the ground. So, the H K theorems essentially what H K theorems do is they reduce the Schrodinger equation. The original Schrodinger equation to finding out the density electron density of the system and from the from by minimizing the energy as a function of the electron density we can find out the ground state energy.

And the ground state is important because that is the state when the system is not interacting with any external agency that is the state that is that gives us the electronic structure the band structure of the system. But they do not tell us about how to calculate the electron density they say these H K theorems tell us that the total energy of the system is and is a functional of electron density.

And the electrons in density that minimizes this energy functional that corresponds to the ground state density. And from the ground state density we can calculate the corresponding ground state wave functions and from there we can calculate all the electronic properties we can calculate all other properties of the system.

So, these theorems are at the heart of the density functional theory and that is why this theory is known as the density functional. Because it deals with the electron density function and it deals and it in this method we the energy is a functional of the electron density that is why density functional theory ok. There are before going into so there is one question that stands here one that is how do we calculate the electron density. How do we calculate this n r at the first place?

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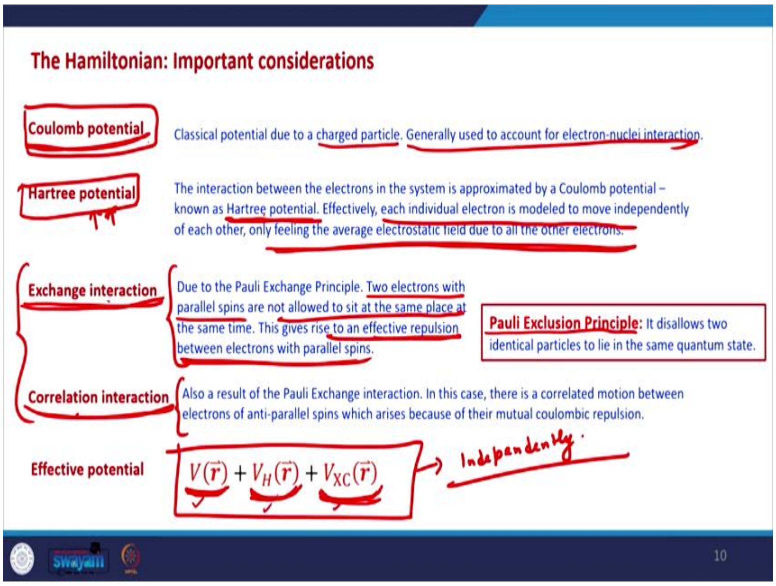

The Hamiltonian: Important considerations

Coulomb potential Classical potential due to a charged particle. Generally used to account for electron-nuclei interaction.

Hartree potential The interaction between the electrons in the system is approximated by a Coulomb potential – known as Hartree potential. Effectively, each individual electron is modeled to move independently of each other, only feeling the average electrostatic field due to all the other electrons.

Exchange interaction Due to the Pauli Exchange Principle. Two electrons with parallel spins are not allowed to sit at the same place at the same time. This gives rise to an effective repulsion between electrons with parallel spins.

Pauli Exclusion Principle: It disallows two identical particles to lie in the same quantum state.

Correlation interaction Also a result of the Pauli Exchange interaction. In this case, there is a correlated motion between electrons of anti-parallel spins which arises because of their mutual coulombic repulsion.

Effective potential $\boxed{V(\vec{r}) + V_H(\vec{r}) + V_{XC}(\vec{r})}$ → Independently.

Before going into that let us have some let us try to understand this multielectron Hamiltonian. Let us try to understand the important parts of the Hamiltonian. So, the first part of the Hamiltonian is the coulomb potential part which is the coulomb potential everybody knows is the classical potential due to a charged particle and it is generally used to account for the electron nuclei interactions. So, it accounts for the interaction of electrons with the atomic course.

Second consideration or second important idea is the idea of Hartree potential. So, that is that lies at the heart of calculating the electron density function. So, what Hartree potential is that we reduce this problem of interacting particles multielectron particles into a problem of non interacting particles.

So, what we do is that this electron electron interaction is effectively reduced or is modeled as an effective potential known as the Hartree potential. And by considering the Hartree potential we can assume that each electron is moving independently of each other just feeling the average electrostatic field which is given by the Hartree potential.

So, this Hartree potential in a way sort of encapsulates the electron electron interaction and it gives us an electrostatic potential or the effective electrostatic potential in which we can assume that the electrons are moving independently of each other. So, this electron electron interaction has been modeled by this Hartree potential .

But there is more to it there is this exchange interaction as well and this exchange interaction comes from the spin properties of the electrons. And in order to understand that we need to understand the or we need to go back to the Pauli's exclusion principle which says that that the two identical spin electrons cannot occupy the same quantum state that in other words what it means is that two electrons of the same spin cannot be at the same place at the same time.

Two electrons of opposite spin can occupy the same orbital, but the two electrons of the same spin cannot occupy the same orbital same state ok. So, the exchange interaction is essentially it due to this principle due to the Pauli's exclusion principle two electrons with parallel spins with identically oriented spins are not allowed to sit at the same place.

This in a way gives rise to an effective repulsion between the electrons of parallel spins. It is not an electrostatic repulsion in a way because electro static repulsion is modeled by the Hartree potential. It is entirely a quantum mechanical kind of interaction that arises because of the Pauli's exclusion principle where two electrons with identical spins cannot be at the same place.

So, effectively it can be termed as or it can be termed as an effective repulsion and also known as the exchange interaction. If repulsion between identical spins electrons please remember that it is different from the coulomb; coulomb interaction it is different from this electrostatic interaction it is origin is in the spins or Pauli's exclusion principle.

Similar way there is this correlation interaction because according to the Pauli's exclusion principle two electrons of opposite spin can be at the same place. But two electrons when they try to come to the same place there will be an electrostatic repulsion. So, they cannot exactly be at the same place.

But there is a sort of correlation between the opposite spins that is purely of quantum mechanical origin and that is modeled by the correlation interaction. So, apart from the coulomb interactions , so this coulomb interaction is coulomb potential is the interaction between electrons and nuclei.

Hartree potential accounts for the electron electron electrostatic interactions and then this exchange and correlation interactions are the they arise from the quantum mechanical properties. They arise from the spin properties of the electrons and governed by the Pauli's exclusion principle.

Effectively they can be written as repulsion forces or correlation forces in a way coupled forces there is a coupling between that there is a coupling between opposite spins and repulsion between the parallel spins. So, finally, the effective potential in a multielectron system can be written as a sum of electron nuclear interactions Hartree potential and exchange correlation term X means exchange, C means correlation.

So, it account for both exchange and correlation and with this we can now say or we can now treat the electrons independently. This interacting electron system can now be treated independently by considering Hartree potential, this electron nuclear coulomb potential and the exchange correlation potential.

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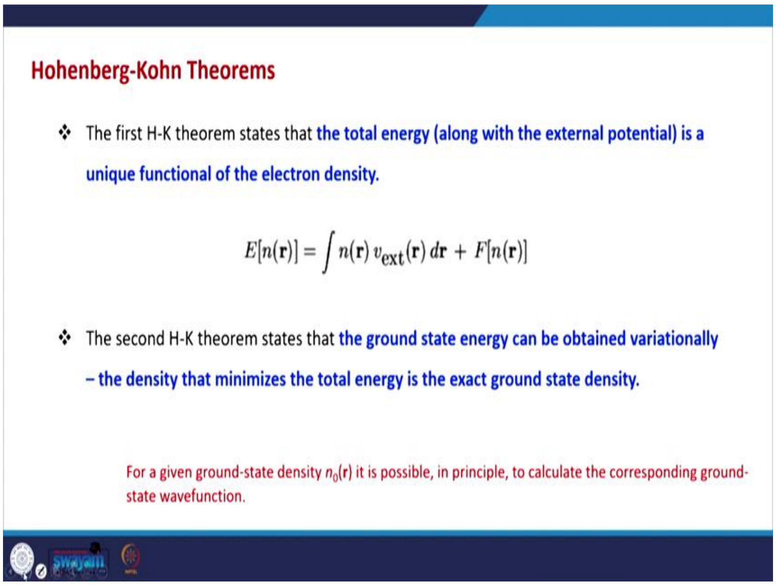

Hohenberg-Kohn Theorems

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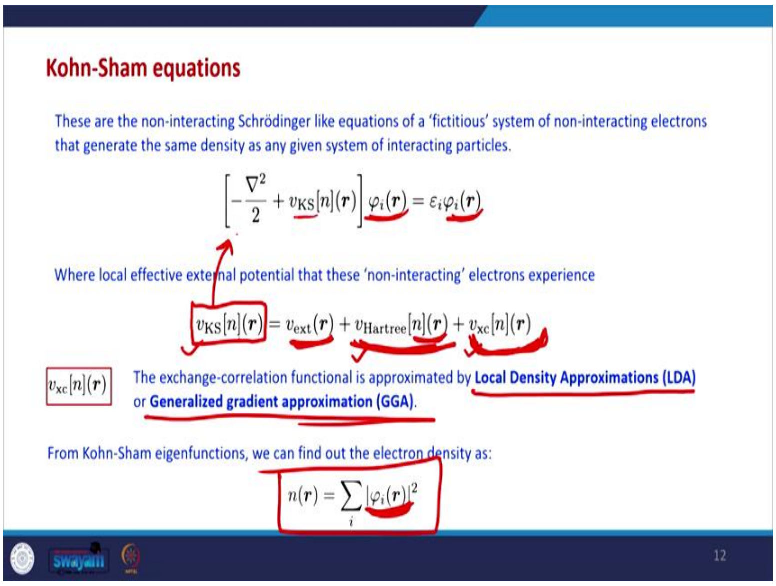

Kohn-Sham equations

These are the non-interacting Schrödinger like equations of a 'fictitious' system of non-interacting electrons that generate the same density as any given system of interacting particles.

$$\left[-\frac{\nabla^2}{2} + v_{\text{KS}}[n](\boldsymbol{r})\right]\varphi_i(\boldsymbol{r}) = \varepsilon_i\varphi_i(\boldsymbol{r})$$

Where local effective external potential that these 'non-interacting' electrons experience

$$\boxed{v_{\text{KS}}[n](\boldsymbol{r})} = v_{\text{ext}}(\boldsymbol{r}) + v_{\text{Hartree}}[n](\boldsymbol{r}) + v_{\text{xc}}[n](\boldsymbol{r})$$

$\boxed{v_{\text{xc}}[n](\boldsymbol{r})}$ The exchange-correlation functional is approximated by **Local Density Approximations (LDA)** or **Generalized gradient approximation (GGA)**.

From Kohn-Sham eigenfunctions, we can find out the electron density as:

$$\boxed{n(\boldsymbol{r}) = \sum_i |\varphi_i(\boldsymbol{r})|^2}$$

With this now we come back to the H K theorems and the thing here was that we do not know how to calculate the electron density function and that problem was solved by Kohn and Sham in 1965 by what is known as the Kohn Sham equations. And Kohn Sham equations are the equations for non interacting electrons in a wave.

So, the electron interacting electrons by using the Hartree potential have been or can be considered to be non-interacting. And we can write down the Schrodinger equation for these this fictitious system for this non interacting system which is an approximation of the interacting system.

But now this potential is modified by the Kohn Sham potential which is essentially the sum of external potential which is electron nuclear interaction Hartree potential which is the effective potential arising out of electron; electron interaction plus this Kohn Sham plus this exchange correlation term.

So, in this method what we do is? We solve the equations or these single particle Schrodinger equations also known as Kohn Sham equations and we calculate the solution of these equations known as the orbital’s phi orbital’s. And if we consider this Kohn Sham potential properly then the electron density can be calculated from these the solution of Kohn Sham equations from the orbital’s phi in this way.

The key point here is that this Kohn Sham potential needs to be properly accounted for and this effective potential that we discussed is essentially the Kohn Sham potential this is. So, this is what we need to properly find out and it has three components the first one is the electron nuclear interaction which is relatively easy to calculate can we can calculate this.

But this second potential the Hartree potential, which is the effective electrostatic potential arising out of electron, electron interaction this depends on the electron density. So, it is also a functional of electron density also the exchange correlation potential is a function of functional of electron density.

The difficult one in this Hartree potential functional is calculated from the Poisson’s equation exchange correlation is a more difficult one and there are multiple approximations to calculate this exchange correlation component. The two most popular ones are the local density approximation LDA or generalized gradient approximations.

So, I am not going into the details of these approximations in this class. But from these we can calculate this exchange correlation component in the Kohn Sham potential functional. This Hartree potential functional can also be calculated from can be calculated from the Poisson equation.

And that way we have this Kohn Sham potential functional and once we have this by solving this single particle Schrodinger equation Kohn Sham equation so called Kohn Sham equation. We can calculate the orbital’s these wave functions and from this we can calculate the electron density.

But again there is a catch here because the density depends on these wave functions Φ’s and the Φ is depend on the solution of this equation. But this equation in this equation this potential functional depends again on n(r) ok.

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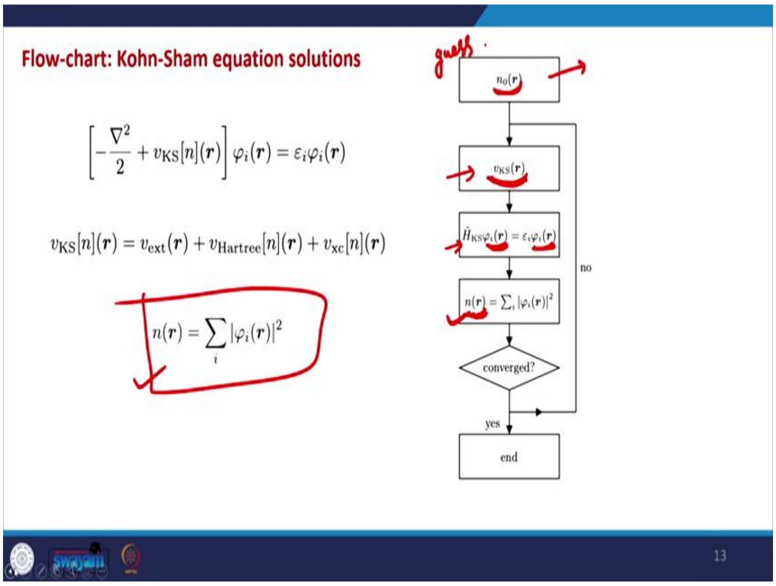

Flow-chart: Kohn-Sham equation solutions

$$\left[-\frac{\nabla^2}{2} + v_{\mathrm{KS}}[n](\boldsymbol{r})\right]\varphi_i(\boldsymbol{r}) = \varepsilon_i\varphi_i(\boldsymbol{r})$$

$$v_{\mathrm{KS}}[n](\boldsymbol{r}) = v_{\mathrm{ext}}(\boldsymbol{r}) + v_{\mathrm{Hartree}}[n](\boldsymbol{r}) + v_{\mathrm{xc}}[n](\boldsymbol{r})$$

$$n(\boldsymbol{r}) = \sum_i |\varphi_i(\boldsymbol{r})|^2$$

So, this is not a closed form again we cannot have a closed form solution for this system of equations and that is why we again need to use the self consistent approach. So, what we do is? We make an initial guess of the electron density from this electron density.

We calculate the Kohn Sham potential functional from this, we calculate the these orbital’s, phi orbital’s. From these orbital’s we again calculate the electron density function and we compare this initial guess this is the first.

We make the guess, we compare $n_0(r)$ with n(r) and if both of them converge then we calculate the final density from this equation. This is the final density of the conversion and from there we can calculate the ground state energy as well according to the H K theorem, second H K theorem.

If they do not converge we again go back and with this new density function. We again calculate the Kohn Sham potential functional. From there we again calculate the Φ values Φ orbital’s, from there we calculate the electron density function. And this process goes on this is known as the self consistent approach to solve the Kohn Sham equations from which we can calculate the electron density function.

So, this in summary is the density functional theory there are and this is a very quick review or very quick introduction to the DFT. And if you are interest this is I would say this is one of the most important calculation method in multiple disciplines nowadays.

So, I would recommend all of you to go back into studying the more details of this method. So, with this we finish this course and as a just to have a quick relook at this course we will see what we have seen so far.

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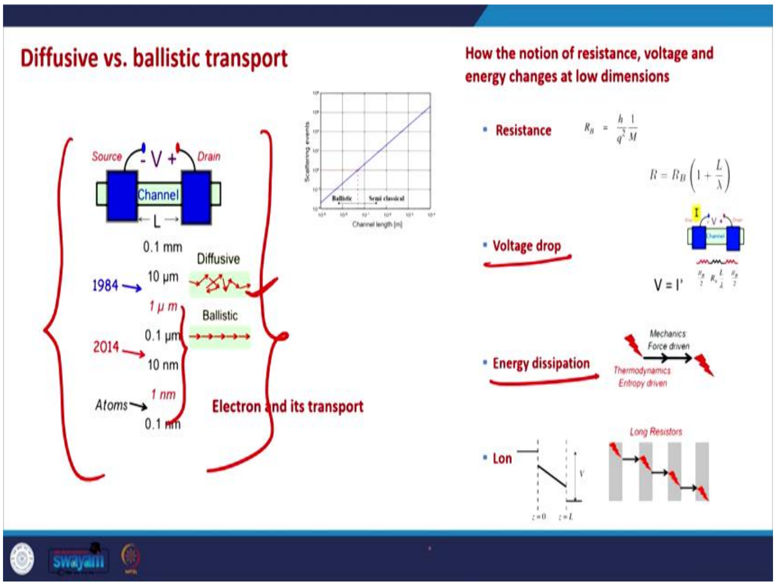

Diffusive vs. ballistic transport

How the notion of resistance, voltage and energy changes at low dimensions

- Resistance $R_B = \frac{h}{q^2}\frac{1}{M}$ $R = R_B\left(1+\frac{L}{\lambda}\right)$
- Voltage drop $V = I'$
- Energy dissipation
- Lon

So, we started with the background why we want to study this kind of course, because and that goes back to the scaling of devices. Because by scaling nowadays the devices are becoming extremely small few tens of nanometers and even some devices are nanostructures nowadays.

So, we and because of this scaling the conventional theory of transport is not sufficient to explain and understand the electronic properties of these devices. They cannot explain the voltage drop in the devices energy dissipation IV characteristics all the things essentially. So, we need to take entirely different approach.

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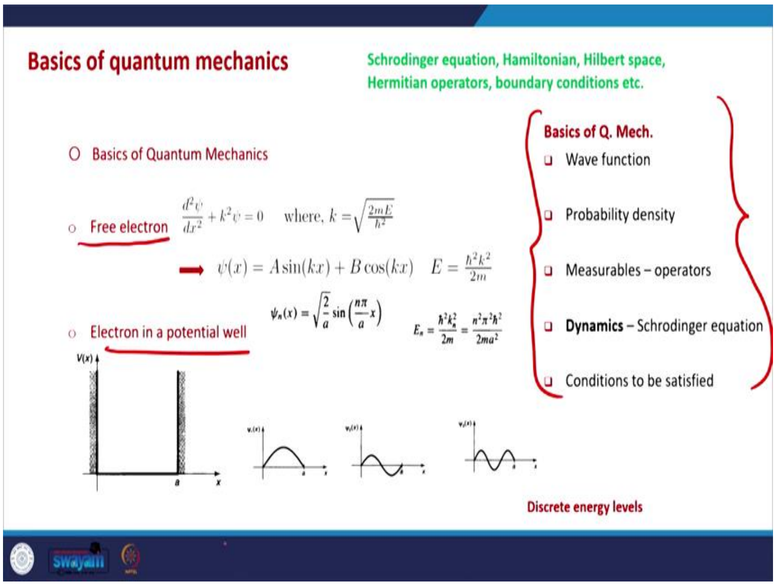

Basics of quantum mechanics

Schrodinger equation, Hamiltonian, Hilbert space, Hermitian operators, boundary conditions etc.

- Basics of Quantum Mechanics
- Free electron $\frac{d^2\psi}{dx^2} + k^2\psi = 0$ where, $k = \sqrt{\frac{2mE}{\hbar^2}}$

$$\Rightarrow \psi(x) = A\sin(kx) + B\cos(kx) \quad E = \frac{\hbar^2 k^2}{2m}$$

- Electron in a potential well $\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$ $E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}$

Basics of Q. Mech.

- ☐ Wave function
- ☐ Probability density
- ☐ Measurables – operators
- ☐ **Dynamics** – Schrodinger equation
- ☐ Conditions to be satisfied

Discrete energy levels

And so that is why we start with the basics of quantum mechanics because in order to understand anything we need to go to the basics. And so in the initial classes we went through the basics of quantum mechanics through the postulates of quantum mechanics then we solved the free electron wave functions.

Then the wave function for electron in a potential way what we see from here is that the confinement of electrons lead to discretization that is a direct consequence of the quantum mechanics.

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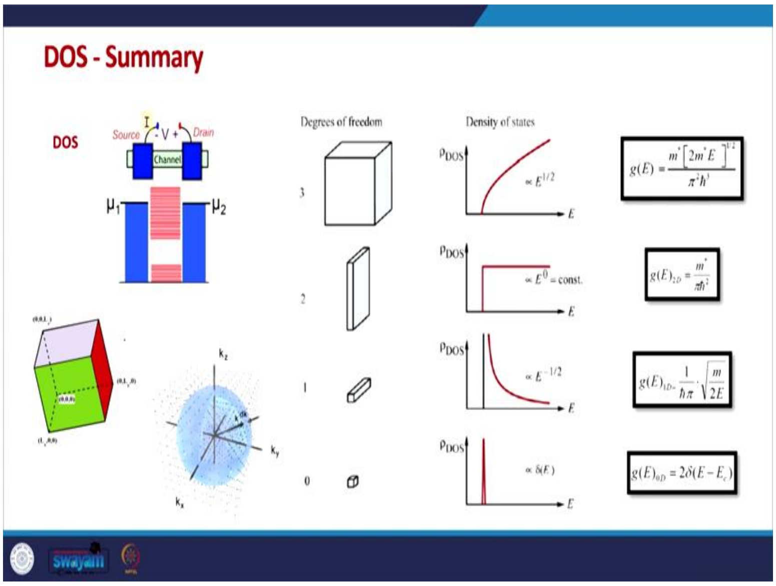

DOS - Summary

$$g(E) = \frac{m^*}{\pi^2\hbar^3}\left[2m^*E\right]^{1/2}$$

$$g(E)_{2D} = \frac{m^*}{\pi\hbar^2}$$

$$g(E)_{1D} = \frac{1}{\hbar\pi}\cdot\sqrt{\frac{m}{2E}}$$

$$g(E)_{0D} = 2\delta(E - E_c)$$

Then we delved into the idea of density of states in the devices especially of the channel. And that we can obtain from the E K relationship between them, we also dealt with the Kronig Penney model or how the electrons behave in solids essentially.

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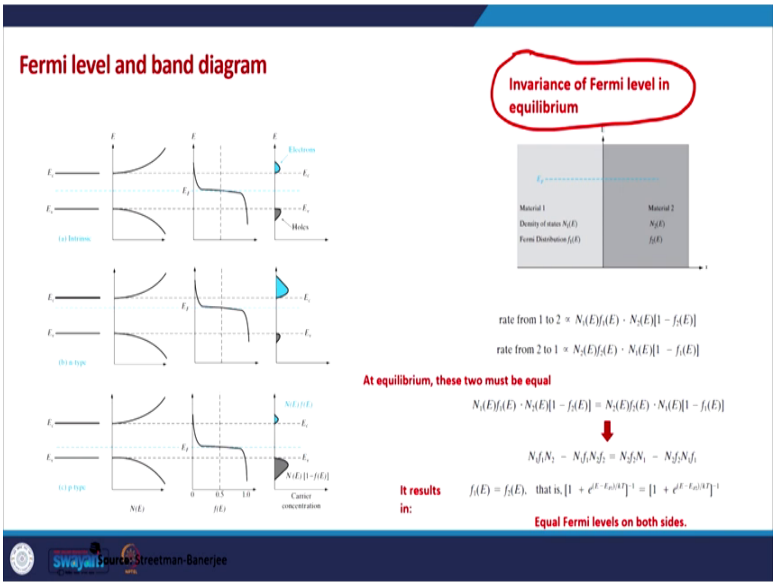

Fermi level and band diagram

Invariance of Fermi level in equilibrium

rate from 1 to 2 $\propto N_1(E)f_1(E)\cdot N_2(E)[1-f_2(E)]$

rate from 2 to 1 $\propto N_2(E)f_2(E)\cdot N_1(E)[1-f_1(E)]$

At equilibrium, these two must be equal

$$N_1(E)f_1(E)\cdot N_2(E)[1-f_2(E)] = N_2(E)f_2(E)\cdot N_1(E)[1-f_1(E)]$$

$$\Downarrow$$

$$N_1f_1N_2 - N_1f_1N_2f_2 = N_2f_2N_1 - N_2f_2N_1f_1$$

It results in: $f_1(E) = f_2(E)$, that is, $[1+e^{(E-E_{F1})/kT}]^{-1} = [1+e^{(E-E_{F2})/kT}]^{-1}$

Equal Fermi levels on both sides.

Source: Streetman-Banerjee

So, after the density of states we try to understand the Fermi level or the idea of Fermi level Fermi distribution function, because in a device generally the channel region is extremely small. So, we need to understand the density of states of the channel. The contacts are bulk we need to understand the Fermi distribution functions. The Fermi levels of the contacts, that is what we did and what we went through is that the Fermi level in equilibrium is invariant across the entire device entire system.

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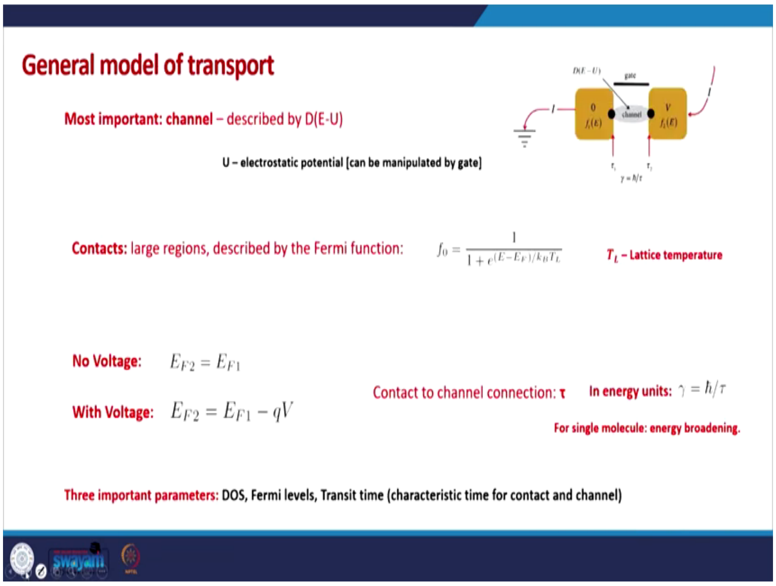

General model of transport

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**

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

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

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

For single molecule: energy broadening.

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

Then we studied the general model of transport which is actually a generalization of Landauer’s model of transport; where the contacts are modeled by the Fermi functions of the contacts and the Fermi levels and the channel is modeled by the density of states.

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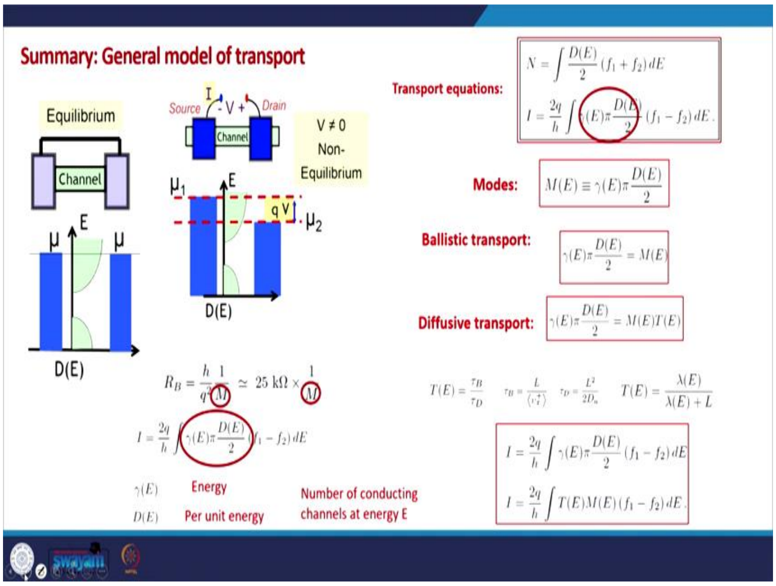

Summary: General model of transport

Transport equations:

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

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

Modes: $M(E) \equiv \gamma(E)\pi\frac{D(E)}{2}$

Ballistic transport: $\gamma(E)\pi\frac{D(E)}{2} = M(E)$

Diffusive transport: $\gamma(E)\pi\frac{D(E)}{2} = M(E)T(E)$

$$R_B = \frac{h}{q^2}\frac{1}{M} \simeq 25\ \text{k}\Omega \times \frac{1}{M}$$

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

$\gamma(E)$ Energy

$D(E)$ Per unit energy

Number of conducting channels at energy E

$T(E) = \frac{\tau_B}{\tau_D}$ $\tau_B = \frac{L}{\langle v_x^+\rangle}$ $\tau_D = \frac{L^2}{2D_n}$ $T(E) = \frac{\lambda(E)}{\lambda(E)+L}$

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

$$I = \frac{2q}{h}\int T(E)M(E)(f_1-f_2)\,dE\,.$$

In the general model of transport we could from this general model of transport we could find out the IV characteristics or the current and the steady state number of electrons. We could also or we came across many new properties as well. For example, the number of modes in a device the broadening of energy levels which is due to the finite lifetime of electrons in a system the notion of the transmission coefficient in a diffusive transport case. This also we came across in the general model of transport.

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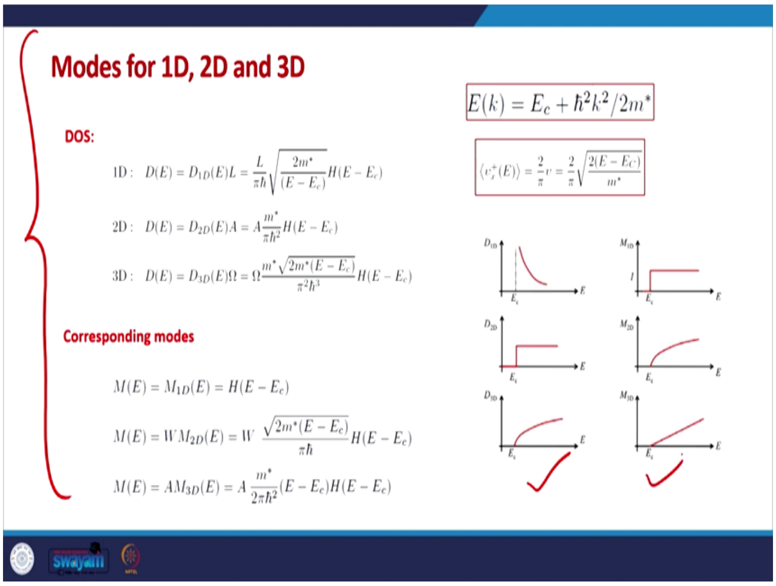

Modes for 1D, 2D and 3D

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

$$\boxed{\langle v_x^+(E)\rangle = \frac{2}{\pi}v = \frac{2}{\pi}\sqrt{\frac{2(E-E_C)}{m^*}}}$$

DOS:

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

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

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

Corresponding modes

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

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

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

Then we studied this idea of modes in great details in all 1D, 2D, 3D devices and compared it to the idea of density of states in 1D, 2D and 3D systems.

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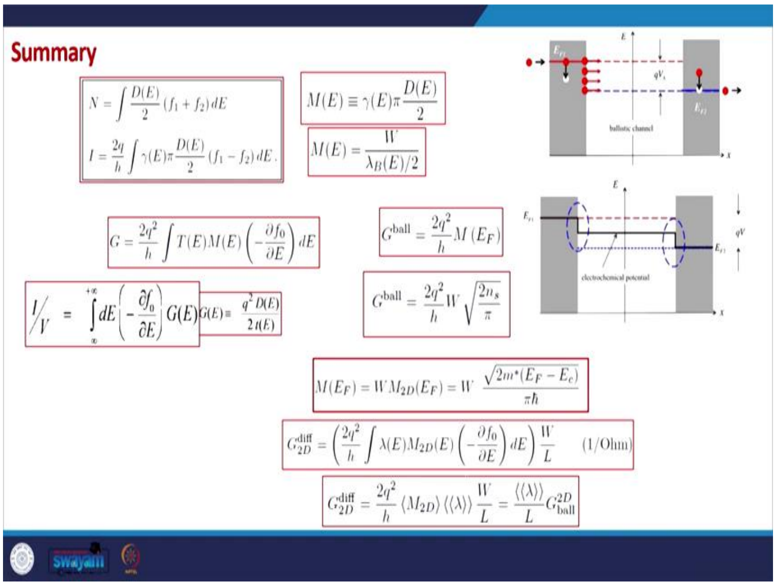

Summary

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

$$\boxed{M(E) \equiv \gamma(E)\pi\frac{D(E)}{2}}$$

$$\boxed{M(E) = \frac{W}{\lambda_B(E)/2}}$$

$$\boxed{G = \frac{2q^2}{h}\int T(E)M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE}$$

$$\boxed{G^{\text{ball}} = \frac{2q^2}{h}M(E_F)}$$

$$\boxed{I/V = \int_{\infty}^{+\infty} dE\left(-\frac{\partial f_0}{\partial E}\right)G(E)} \boxed{G(E) \equiv \frac{q^2 D(E)}{2t(E)}}$$

$$\boxed{G^{\text{ball}} = \frac{2q^2}{h}W\sqrt{\frac{2n_s}{\pi}}}$$

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

$$\boxed{G_{2D}^{\text{diff}} = \left(\frac{2q^2}{h}\int \lambda(E)M_{2D}(E)\left(-\frac{\partial f_0}{\partial E}\right)dE\right)\frac{W}{L} \qquad (1/\text{Ohm})}$$

$$\boxed{G_{2D}^{\text{diff}} = \frac{2q^2}{h}\langle M_{2D}\rangle\langle\langle\lambda\rangle\rangle\frac{W}{L} = \frac{\langle\langle\lambda\rangle\rangle}{L}G_{\text{ball}}^{2D}}$$

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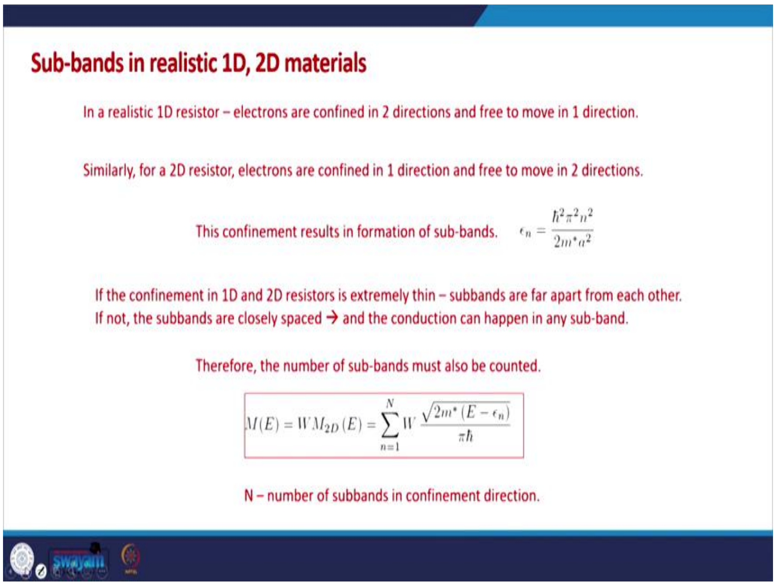

Sub-bands in realistic 1D, 2D materials

In a realistic 1D resistor – electrons are confined in 2 directions and free to move in 1 direction.

Similarly, for a 2D resistor, electrons are confined in 1 direction and free to move in 2 directions.

This confinement results in formation of sub-bands. $\epsilon_n = \frac{\hbar^2 \pi^2 n^2}{2m^* a^2}$

If the confinement in 1D and 2D resistors is extremely thin – subbands are far apart from each other.
If not, the subbands are closely spaced → and the conduction can happen in any sub-band.

Therefore, the number of sub-bands must also be counted.

$$\boxed{M(E) = W M_{2D}(E) = \sum_{n=1}^{N} W \frac{\sqrt{2m^* (E - \epsilon_n)}}{\pi \hbar}}$$

N – number of subbands in confinement direction.

Then we tried to understand the notion of voltage drop and energy dissipation in ballistic transport. And we calculated various device parameters for a 2 terminal device from the general model of transport. The important one is this calculation of conductance in near equilibrium transport case and we did this calculation for multiple different temperatures different materials.

Then we had a discussion on the sub bands in 1D and 2D materials. Because in practice 1D and 2D materials are not actual 1D, 2D materials, they are quasi 1D and quasi 2D materials. So, electrons can move in one direction freely, but confined in other 2 directions in 1D materials.

Similarly in 2D materials electrons can move in two directions confined in the third material and that is why in the this confined direction energy states become discrete and we need to consider the sub bands because of these discrete energy levels.

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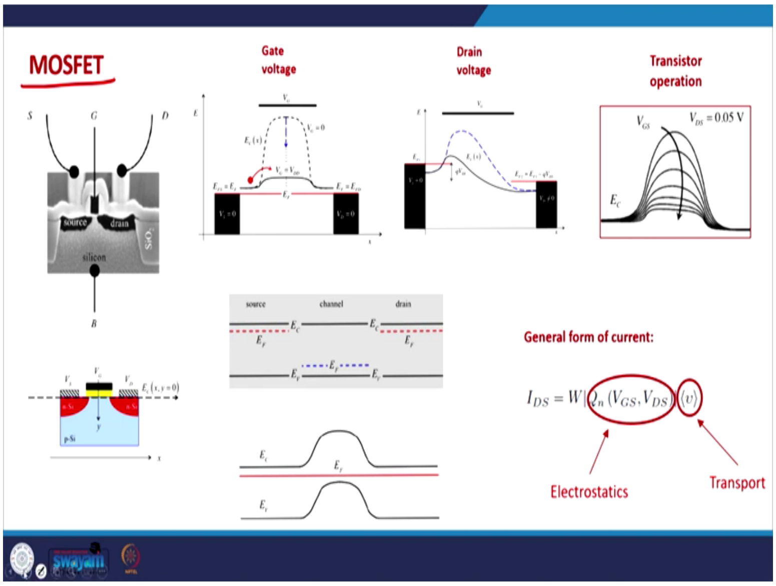

MOSFET

General form of current:

$$I_{DS} = W|Q_n(V_{GS}, V_{DS})|\langle v\rangle$$

Electrostatics

Transport

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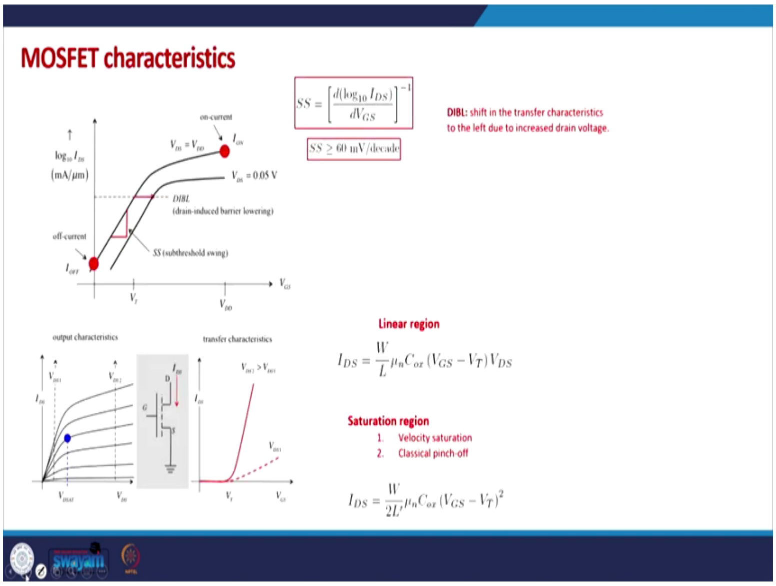

MOSFET characteristics

$$SS = \left[\frac{d(\log_{10} I_{DS})}{dV_{GS}}\right]^{-1}$$

$$SS \geq 60 \text{ mV/decade}$$

DIBL: shift in the transfer characteristics to the left due to increased drain voltage.

Linear region

$$I_{DS} = \frac{W}{L}\mu_n C_{ox}(V_{GS} - V_T)V_{DS}$$

Saturation region

1. Velocity saturation
2. Classical pinch-off

$$I_{DS} = \frac{W}{2L}\mu_n C_{ox}(V_{GS} - V_T)^2$$

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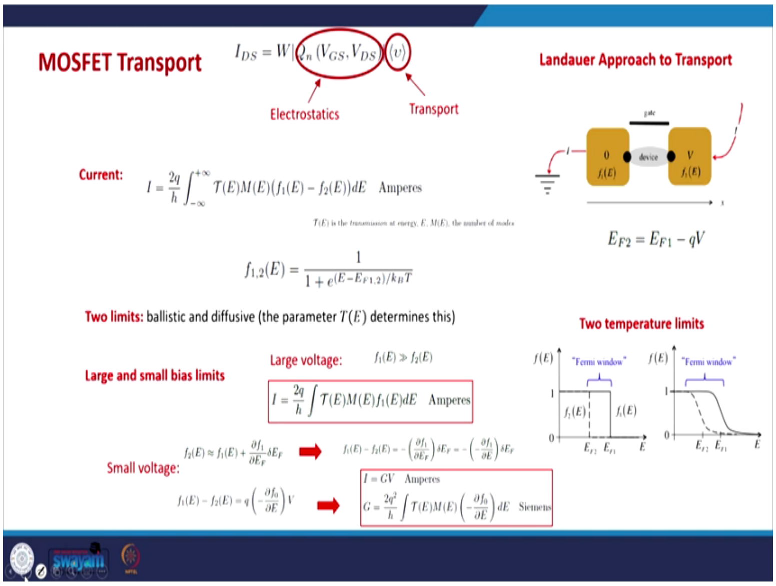

MOSFET Transport

$I_{DS} = W|Q_n(V_{GS}, V_{DS})|\langle v \rangle$

Electrostatics

Transport

Landauer Approach to Transport

Current: $I = \frac{2q}{h}\int_{-\infty}^{+\infty} \mathcal{T}(E)M(E)(f_1(E) - f_2(E))dE$ Amperes

$\mathcal{T}(E)$ is the transmission at energy, E, $M(E)$, the number of modes

$$f_{1,2}(E) = \frac{1}{1 + e^{(E - E_{F1,2})/k_BT}}$$

$$E_{F2} = E_{F1} - qV$$

Two limits: ballistic and diffusive (the parameter $\mathcal{T}(E)$ determines this)

Two temperature limits

Large and small bias limits

Large voltage: $f_1(E) \gg f_2(E)$

$$\boxed{I = \frac{2q}{h}\int \mathcal{T}(E)M(E)f_1(E)dE \quad \text{Amperes}}$$

Small voltage:

$f_2(E) \approx f_1(E) + \frac{\partial f_1}{\partial E_F}\delta E_F \Rightarrow f_1(E) - f_2(E) = -\left(\frac{\partial f_1}{\partial E_F}\right)\delta E_F = -\left(-\frac{\partial f_1}{\partial E}\right)\delta E_F$

$f_1(E) - f_2(E) = q\left(-\frac{\partial f_0}{\partial E}\right)V \Rightarrow$

$$\boxed{\begin{array}{l} I = GV \quad \text{Amperes} \\ G = \frac{2q^2}{h}\int \mathcal{T}(E)M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE \quad \text{Siemens} \end{array}}$$

So, that is what we discussed then we tried to we went to understand the 3 terminal devices. Essentially the MOSFET device which is the main component of electronic devices. In today's world, we try to understand the IV characteristics of the MOSFET.

We had a discussion on the conventional MOSFET theory, in the beginning then we went to the MOSFET transport theory. We applied the general model of transport on the three terminal device on the MOSFET's.

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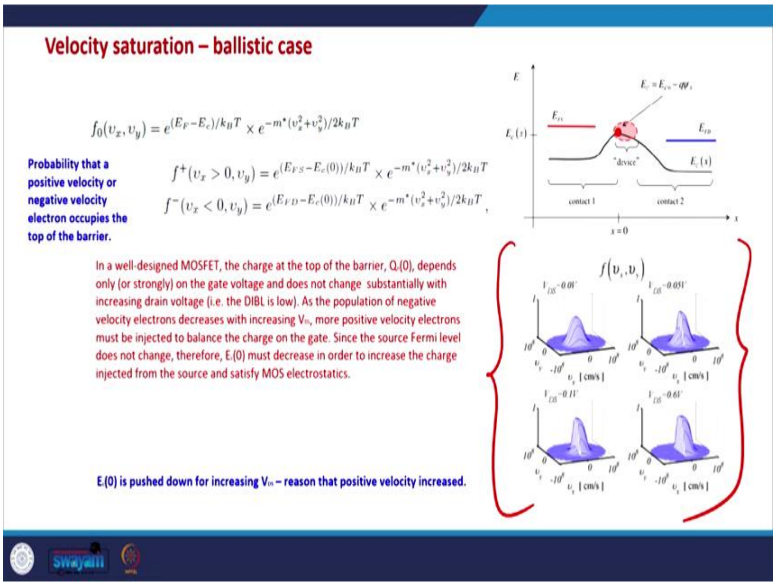

Velocity saturation – ballistic case

$$f_0(v_x, v_y) = e^{(E_F - E_c)/k_BT} \times e^{-m^*(v_x^2 + v_y^2)/2k_BT}$$

Probability that a positive velocity or negative velocity electron occupies the top of the barrier.

$$f^+(v_x > 0, v_y) = e^{(E_{FS} - E_c(0))/k_BT} \times e^{-m^*(v_x^2 + v_y^2)/2k_BT}$$

$$f^-(v_x < 0, v_y) = e^{(E_{FD} - E_c(0))/k_BT} \times e^{-m^*(v_x^2 + v_y^2)/2k_BT},$$

In a well-designed MOSFET, the charge at the top of the barrier, $Q_n(0)$, depends only (or strongly) on the gate voltage and does not change substantially with increasing drain voltage (i.e. the DIBL is low). As the population of negative velocity electrons decreases with increasing V_{DS}, more positive velocity electrons must be injected to balance the charge on the gate. Since the source Fermi level does not change, therefore, $E_c(0)$ must decrease in order to increase the charge injected from the source and satisfy MOS electrostatics.

$E_c(0)$ is pushed down for increasing V_{DS} – reason that positive velocity increased.

What we could see is this is this was one of the most important discussions in the MOSFET transport; that MOSFET is a barrier control device. So, there is a barrier from the source to the drain in the MOSFET and the velocity at the top of barrier is very important. And we try to understand the saturation of velocity in ballistic MOSFET.

So, in general MOSFET's the velocity saturates because of the collisions. But in ballistic MOSFET's it is not due to collision. It is because of the it comes from the electronic structure distribution of velocities in MOSFET at the top of the barrier. So, that is what we discussed.

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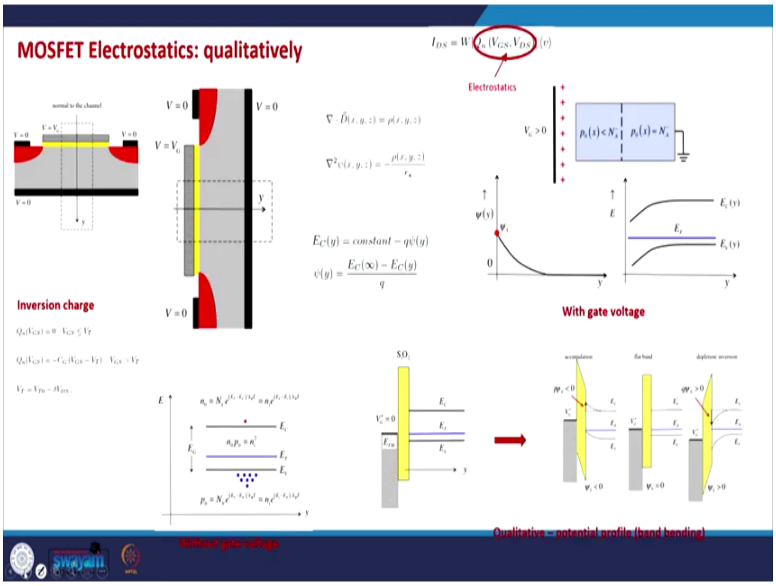

MOSFET Electrostatics: qualitatively

$I_{DS} = W Q_n(V_{GS}, V_{DS}) \langle v \rangle$

Electrostatics

$\nabla \cdot \vec{D}(x,y,z) = \rho(x,y,z)$

$\nabla^2 \psi(x,y,z) = -\frac{\rho(x,y,z)}{\epsilon_s}$

$E_C(y) = constant - q\psi(y)$

$\psi(y) = \frac{E_C(\infty) - E_C(y)}{q}$

Inversion charge

$Q_n(V_{GS}) = 0 \quad V_{GS} \le V_T$

$Q_n(V_{GS}) = -C_G(V_{GS} - V_T) \quad V_{GS} > V_T$

$V_T = V_{T0} - \delta V_{DS}$

With gate voltage

Without gate voltage

Qualitative – potential profile (band bending)

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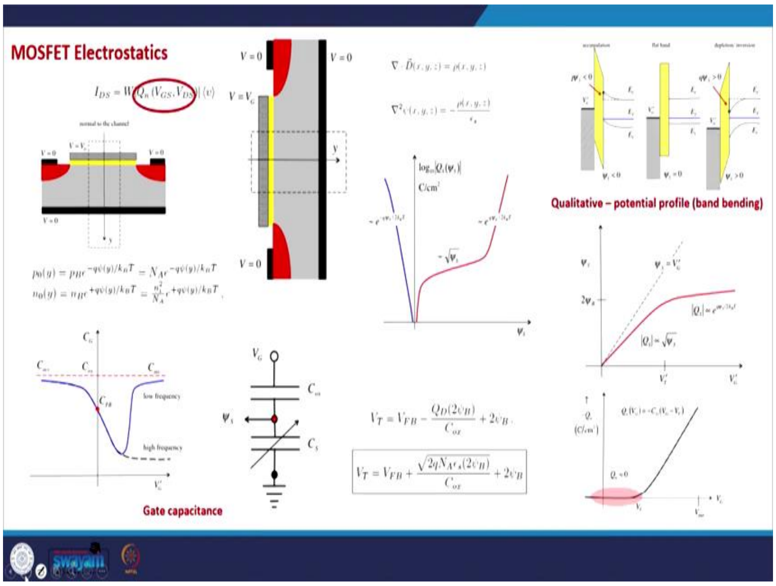

MOSFET Electrostatics

$I_{DS} = W Q_n(V_{GS}, V_{DS}) \langle v \rangle$

$p_0(y) = p_B e^{-q\psi(y)/k_BT} = N_A e^{-q\psi(y)/k_BT}$

$n_0(y) = n_B e^{+q\psi(y)/k_BT} = \frac{n_i^2}{N_A} e^{+q\psi(y)/k_BT}$

$\nabla \cdot \vec{D}(x, y, z) = \rho(x, y, z)$

$\nabla^2 \psi(x, y, z) = -\frac{\rho(x, y, z)}{\epsilon_s}$

$V_T = V_{FB} - \frac{Q_D(2\psi_B)}{C_{ox}} + 2\psi_B$

$$\boxed{V_T = V_{FB} + \frac{\sqrt{2qN_A\epsilon_s(2\psi_B)}}{C_{ox}} + 2\psi_B}$$

Gate capacitance

Qualitative – potential profile (band bending)

Then we went to understand the MOSFET electrostatics first. The conventional MOSFET electrostatics we had a detailed discussion on the charge in the semiconductor as a function of the semi conductor potential relationship between the semi conductor potential at the interface to the gate voltage the relationship between the mobile charge and the gate voltage.

We could also understand the notion of the threshold voltage which is the voltage. The gate voltage at which the inversion happens we also delved into the idea of gate capacitance which is essentially has two components in series. One is the oxide capacitance and second is the semiconductor capacitance we discussed this both at low frequency and high frequency.

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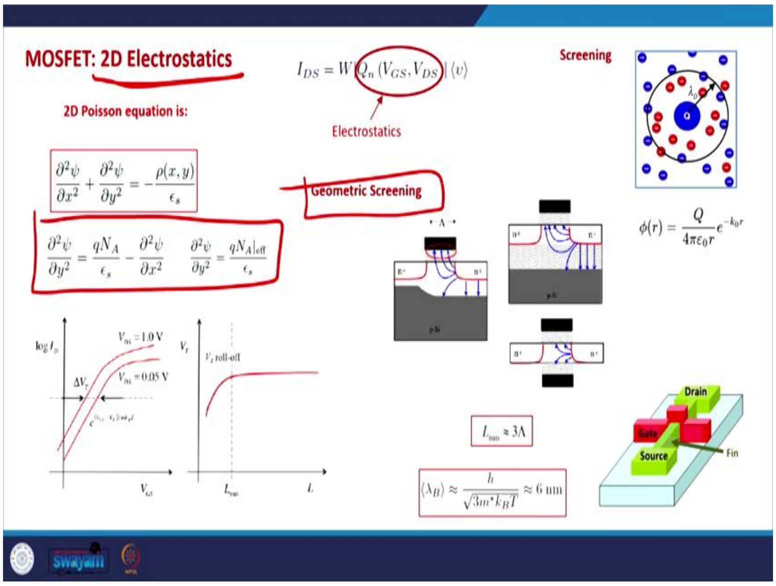

MOSFET: 2D Electrostatics

$$I_{DS} = W\,|Q_n(V_{GS}, V_{DS})|\,\langle v\rangle$$

Electrostatics

2D Poisson equation is:

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} = -\frac{\rho(x,y)}{\epsilon_s}$$

$$\frac{\partial^2\psi}{\partial y^2} = \frac{qN_A}{\epsilon_s} - \frac{\partial^2\psi}{\partial x^2} \qquad \frac{\partial^2\psi}{\partial y^2} = \frac{qN_A|_{\text{eff}}}{\epsilon_s}$$

Geometric Screening

Screening

$$\phi(r) = \frac{Q}{4\pi\varepsilon_0 r}e^{-k_0 r}$$

$$L_{\min} \approx 3\Lambda$$

$$\langle\lambda_B\rangle \approx \frac{h}{\sqrt{3m^* k_B T}} \approx 6\text{ nm}$$

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Then we discussed this important consideration in MOSFET electrostatics which is the 2D electrostatics which is prominent in modern day nanoscale devices. And what we saw was that because of this 2D electrostatic effects the threshold voltage is reduced or the gate control is reduced on the channel.

And as a method of countering this these 2D electrostatic effects we discussed the idea of geometric screening which is done by surrounding the channel with the gate on multiple sides ok.

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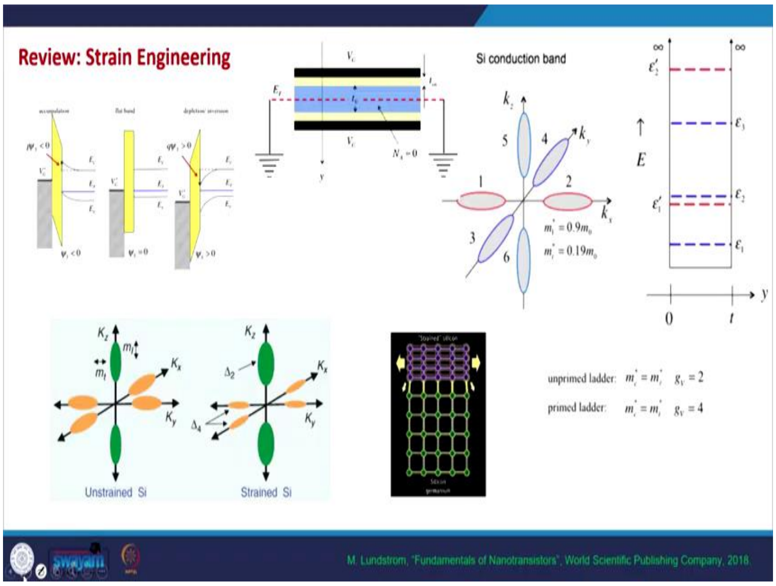

Review: Strain Engineering

Si conduction band

$m_l^* = 0.9m_0$

$m_t^* = 0.19m_0$

unprimed ladder: $m_y^* = m_l^*$ $g_V = 2$

primed ladder: $m_y^* = m_t^*$ $g_V = 4$

M. Lundstrom, "Fundamentals of Nanotransistors", World Scientific Publishing Company, 2018.

So, after the 2D electrostatics we had a discussion on the strain engineering. How this strain can enhance the performance strain applied in certain directions can enhance the performance the better current in a nano transistor.

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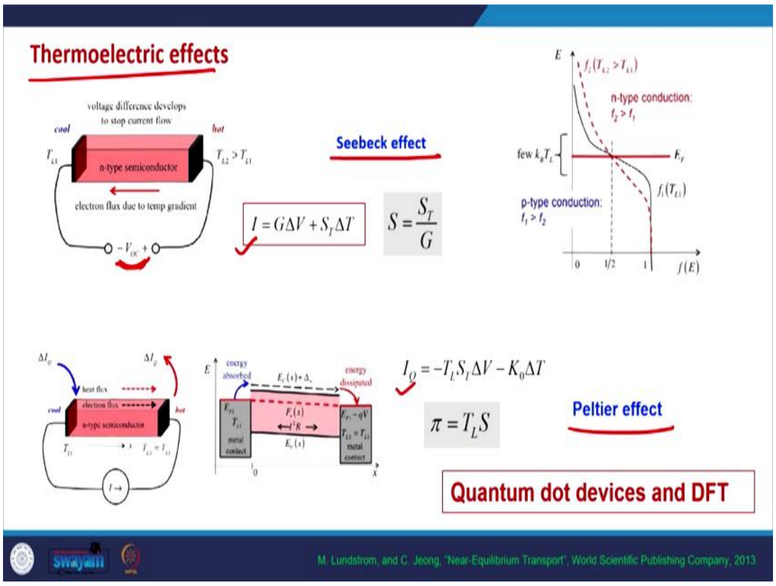

Thermoelectric effects

Seebeck effect

$$I = G\Delta V + S_T \Delta T$$

$$S = \frac{S_T}{G}$$

$$I_Q = -T_L S_T \Delta V - K_0 \Delta T$$

$$\pi = T_L S$$

Peltier effect

Quantum dot devices and DFT

M. Lundstrom, and C. Jeong, "Near-Equilibrium Transport", World Scientific Publishing Company, 2013

Then we delve into we discussed the thermoelectric effects prominently two effects one is the Seebeck effect and second is the Peltier effect. We discussed the notion of charge current and heat current Seebeck effect essentially relates to the development of or because of the temperature difference voltage is developed across a semiconductor.

The reverse happens in the case of Peltier effect because of a current flow in a semiconductor the heat current also flows which develops a temperature difference. So, that is what we discussed in thermoelectric effects and derived the Seebeck coefficient and Peltier coefficient. And in last few classes we have been discussing the quantum dot devices and we have a very short and quick introduction on the density function theory.

So, that is essentially what we what was the subject matter of this course. I hope all of you enjoyed this course if you have any feedback about the course please give it to me either on my email ID or on the course page. And finally, I would again thank you for enrolling for this course.

Thank you.