Physics of Nanoscale Devices
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Lecture - 14
DOS, Fermi Function

Hello everyone. Today, we will conclude our discussion of Density of States and we will start a new topic called Fermi Function or Fermi Dirac Distribution Function, which essentially means the probability of a state being occupied.

But let us first wrap up what we were discussing about the density- of states and this is what we have covered so far; the density of states in a material is essentially the states available for conduction the electronic states available for conduction. So, these are the unique electronic states, distinct electronic states available in a material which the electron can occupy, if it has the required energy.

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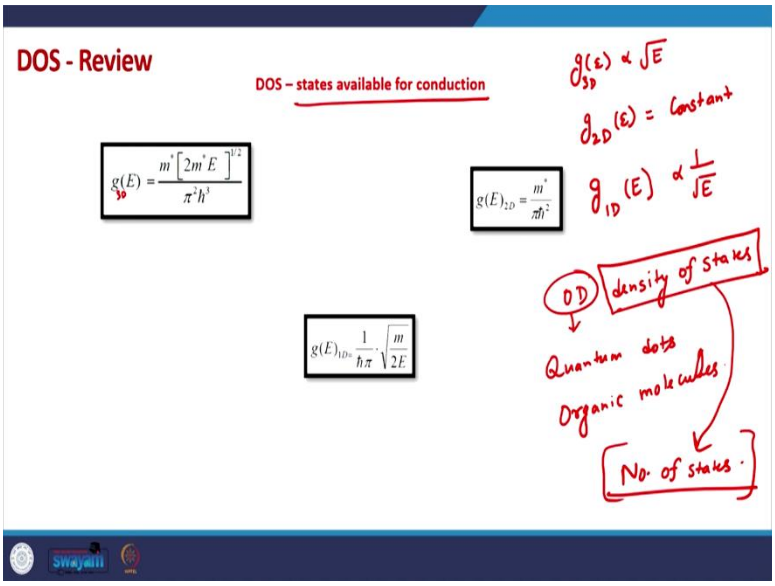

DOS - Review

DOS – states available for conduction

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

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

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

$g_{3D}(\varepsilon) \propto \sqrt{E}$

$g_{2D}(\varepsilon) =$ Constant

$g_{1D}(E) \propto \frac{1}{\sqrt{E}}$

0D density of states

Quantum dots

Organic molecules.

No. of states.

And for the 3D material we saw that g_{3D} is essentially directly proportional to square root of E. A 2D density of states is constant; it is not a function of energy, it is independent of the energy of the electrons. It is a constant value given by $\frac{m^*}{\pi\hbar^2}$. And 1D density of states is inversely related to the energy in this way; square root of 1 by square root E. During the end of last lecture, I asked you to think about 0D density of states; what would be the density of states for a 0D material?

So, a 0D material is essentially a material in which electrons are confined like they are confined in an atom basically, so or in a molecule. So, example of 0D materials are quantum dots, as I have repeatedly discussed organic molecules.

By the way, organic molecules are nowadays being used in many novel electronic devices for their application. For example, the DNA molecules are being tested for their electronic properties and in some devices, they find interesting applications.

So, the organic molecules and quantum dots are example of 0D material and a 0D material is essentially a big molecule. It is a single molecule or it might be a single molecule or it might be a combination of atoms making it a macromolecule; but it is like a molecule. So, in this case, what would be the density of states? That is the question that is there.

So, in order to answer this question, we need to see so as you might recall that in order to find out the density of states, we need to count the number of states essentially and for that, we need to see how electronic states are distributed in a material basically ok. So, how are electronic states distributed in an atom or in a molecule? Just think about it.

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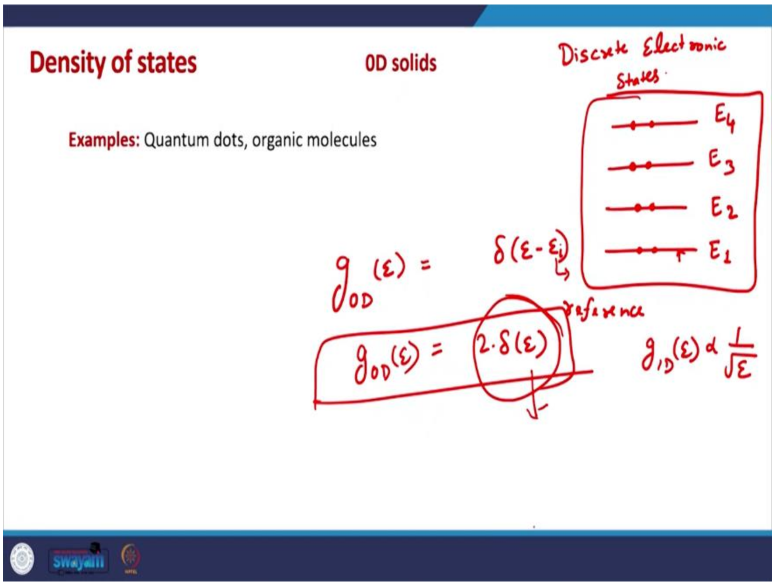

Density of states

0D solids

Examples: Quantum dots, organic molecules

Discrete Electronic States.

$g_{0D}(\varepsilon) = \quad \delta(\varepsilon - \varepsilon_i)$

reference

$$\boxed{g_{0D}(\varepsilon) = 2\cdot\delta(\varepsilon)}$$

$g_{1D}(\varepsilon) \propto \frac{1}{\sqrt{\varepsilon}}$

In a 0D atom, in a 0D solids and the answer is simple that there are discrete electronic states. So, if we plot the states in an atom, this is how it looks like. The confinement in all directions causes discretization of electronic states.

In 1D solids as we have already seen that 1D solids might have bands and band gaps; 2D solids again might have bands and band gaps; 3D solids might also have bands and band gaps; but of 0D solid the electronic states will be discretely placed. Because the electron is confined in all directions and confinement leads to discretization of energy and this is how the electronic states would look like.

So, in a very simple term, we can write down the density of states for 0D material to be delta function essentially ok; where, E_i corresponds to the band or corresponds to a reference energy level and if you take the reference to be 0, it will just be delta times E.

But here also each of these electronic states can occupy up to 2 electrons because the electrons can have up spin and down spin and as we already know that opposite spin electrons can stay in one energy level that would make their quantum numbers different, at least the spin quantum number different and that would not violate any physical principle.

So, this is the density of states in 0D material. It is as simple as that because there is no volume in 1D in 0D solids and then, electronic states per unit volume per unit energy can just be given by this delta function. So, as you might have seen in 1D case, let us say the density of states is inversely proportional to the square root of energy.

So, if we plot the density of states as a function of energy in 1D case, what do you expect? It would be a decreasing function because as the E value increases, the density of state function decreases.

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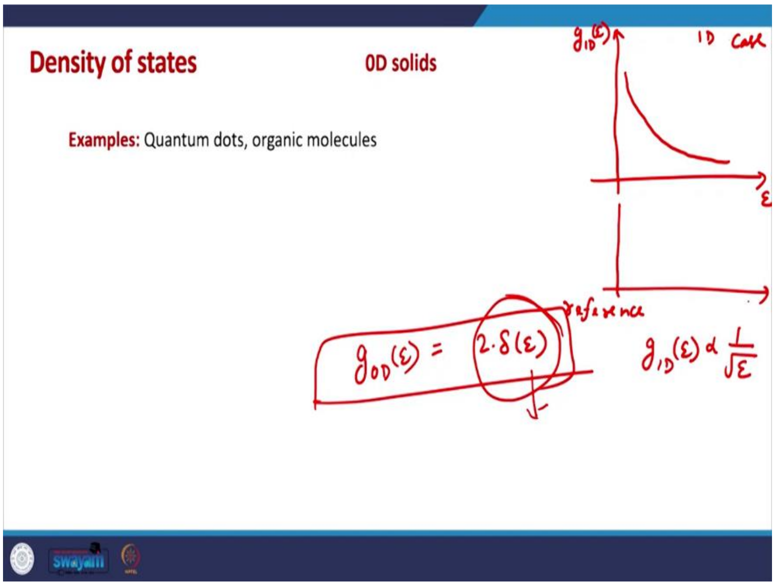

Density of states

0D solids

Examples: Quantum dots, organic molecules

$g_{0D}(\varepsilon) = 2\cdot\delta(\varepsilon)$

$g_{1D}(\varepsilon) \propto \frac{1}{\sqrt{\varepsilon}}$

So, this g(E) function will be a for 1D case, $g_{1D}(E)$ as a function of E, it would be a decreasing kind of function like this. For when energy values are very less, it will have a large the density of states would be large number. As the energy value goes to higher values, this will be a small number.

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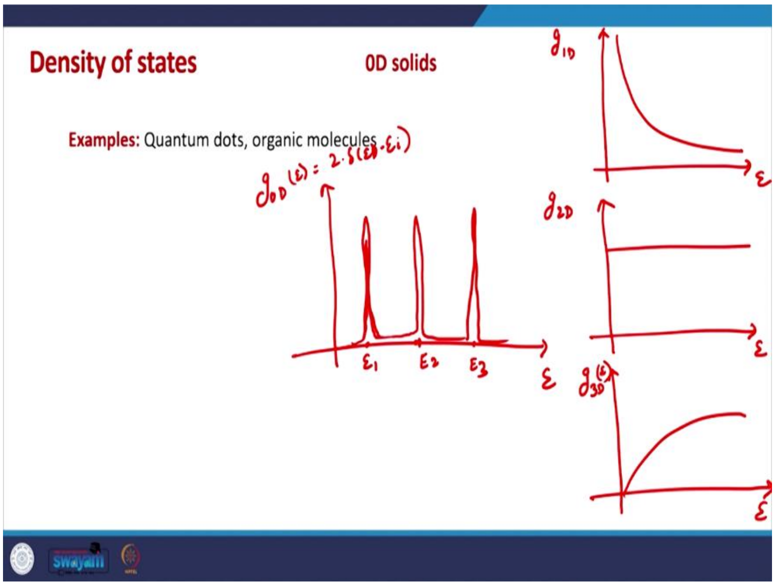

Density of states

0D solids

Examples: Quantum dots, organic molecules

$g_{0D}(\varepsilon) = 2\cdot\delta(\varepsilon-\varepsilon_i)$

And if you recall for 2D cases, the density of states is. For 1D, it is like this; for 2D case, $g_{2D}(E)$ as a function of energy is essentially for 2D case, it is constant; for 3D case, it is an increasing function; $g_{3D}(E)$ and for 0D case, it is just a delta function.

So, corresponding to different or I would say $\partial(E - E_i)$, where these can be different energy values, corresponding to different allowed energy values, it will be a delta function like this. It will have a peak at all these peaks will be of same height. So, if this is first allowed electronic state, this is second, if this is third, like this ok.

So, now, we sort of know how density of states look like in 3D, 2D, 1D and 0D materials. Now, we are ready to sort of ready to understand how to use the density of states idea in our electronic devices. So, for that, we also need to understand this is the summary of density of states. This we have already seen that for 3D case, increasing function; 2D case, constant function; 1D case, decreasing function and 0D case, it is a delta function ok.

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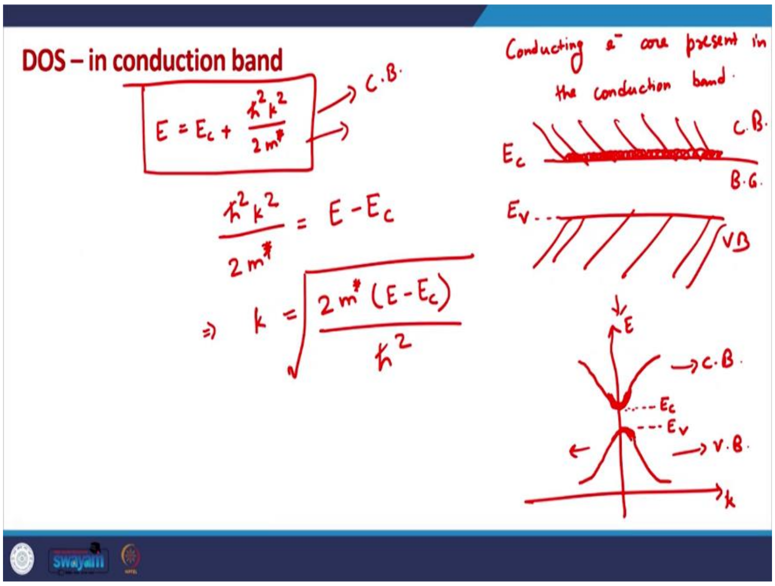

DOS – in conduction band

$$\boxed{E = E_c + \frac{\hbar^2 k^2}{2m^*}} \rightarrow C.B.$$

$$\frac{\hbar^2 k^2}{2m^*} = E - E_c$$

$$\Rightarrow k = \sqrt{\frac{2m^*(E - E_c)}{\hbar^2}}$$

Conducting e^- are present in the conduction band.

Generally, in solids conduction or conducting electrons are present in the conduction band. So, generally in solids, if this is the band structure, if this is the valence band, most of these states are filled. If this is the conduction band in between there is a band gap, this is conduction band, there will be a small number of electrons at the bottom of the conduction band and the energy value at the top of the valence band is popularly written as Ev; the energy at the bottom of the conduction band is written as Ec.

The corresponding E k diagram for this is this we have also seen in our earlier classes, especially during the discussion of KP model, this is the actual this is how the actual E k diagram looks like.

This is the valence band; this is the conduction; this is the among the simplest E k diagram for conduction band and valence bands basically and at the top of the valence band and at the bottom of the conduction band, generally the E k relationship is parabolic. So, that is why we can use the use the parabolic relationship.

We can use this parabolic relationship $\frac{\hbar^2 k^2}{2m^*}$ But if this energy value, if this value is the bottom of the conduction band reference energy value is Ec, in this case the E k relationship between the E k relationship for electrons at the bottom of the conduction band would be E equals Ec + $\frac{\hbar^2 k^2}{2m^*}$.

So, we need to add this reference value in the E k relationship. This is the E k in solids in devices generally this is the E k relationship that we will use for electrons in conduction band. Similarly, in valence band if this energy level is Ev the E k relationship would look like E equals Ev - $\frac{\hbar^2 k^2}{2m^*}$.

Generally, we are mostly concerned about the electrons at the bottom of the conduction band because those are the major contributors in conduction, specially in doped semiconductors ok. So, that is why we will use this relationship in most of our device analysis.

So, with this relationship, the density of states would change a little bit; the expression for the density of states would change a little bit because now, this $\frac{\hbar^2 k^2}{2m^*}$ will be E - Ec. So, which means k will be now $\frac{\sqrt{2m^*(E-Ec)}}{\hbar}$.

So, instead of E, we will have a factor of E minus Ec in all our expressions, especially in density of states. So, the density of states for 3D material in conduction band the form will be the same; but in place of E, we will have E - Ec essentially. Similarly, in 2D, 1D and 0D cases as well. If 0D kind of situation is arising in the conduction.

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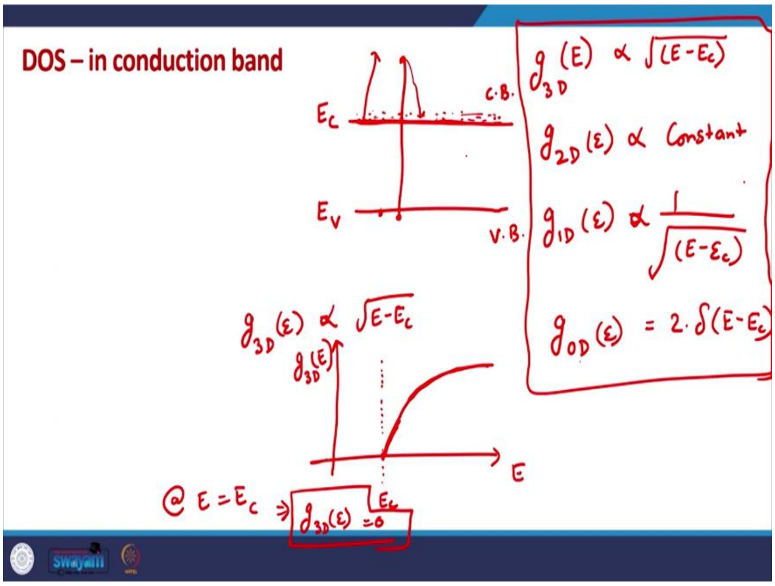

DOS – in conduction band

$g_{3D}(E) \propto \sqrt{(E-E_c)}$

$g_{2D}(\varepsilon) \propto$ Constant

$g_{1D}(\varepsilon) \propto \frac{1}{\sqrt{(E-\varepsilon_c)}}$

$g_{0D}(\varepsilon) = 2 \cdot \delta(E-E_c)$

$g_{3D}(\varepsilon) \propto \sqrt{E-E_c}$

@ $E = E_c \Rightarrow \boxed{g_{3D}(\varepsilon) = 0}$

But in 3D case, this E k relationship, this g_{3D}(E) would be directly proportional to the square root of E –Ec; g_{2D}(E) will still be constant because it was already independent of energy and g_{1D} will be inversely proportional to square root of E - Ec.

Similarly, for a 0D material, we can write it to be delta function at Ec or $2\partial(E - Ec)$. So, these are the density of states expression in conduction band of most of the in semiconductors that is what we will use in our analysis and now, there is an interesting observation that we can make from these expressions.

So, if we plot in a material, if we plot for example, if this is the conduction band, this is Ec bottom of the conduction band. If this is the top of the valence band Ev, so the valence band is here, conduction band is here; this is the band gap.

Now, for a 3D material, if the channel is a 3D material, in that case g_{3D}(E) in conduction band would be directly proportional to square root of E - Ec. What it says is that the plot of density of states in 3D material in conduction band as a function of energy will now slightly be shifted to the edge of the conduction.

So, if this is the conduction band energy Ec, this point is Ec, so this function would be plotted as this. So, at E equals to E c, g_{3D}(E) would be 0. So, what it says is that if we are using a 3D channel, in a 3D channel at the bottom of the conduction band, right at the bottom of the conduction band, the density of states is 0.

So, what it says is that no electron can exist at the edge of the conduction band in a 3D solid because the density of state is 0 at the edge of the conduction band and as we go above conduction band edge, as we go above from the bottom of the conduction band, the density of states is increased.

So, the number of allowed electronic states around the bottom of the conduction band in this range here in this area so to say in this regime will be less. So, the number of electrons that exist in very close to the bottom of conduction band will be a small number in 3D devices.

That is an important thing because generally, the perception that we have is that an electron goes from the top of the valence band to the bottom of the conduction band or a electron goes from the valence band to a higher energy and then, it relaxes the energy and comes down to the bottom of the conduction band.

But in a 3D channel which is and 3D channels are among the most common channels that we use. 3D material, just at the edge of the conduction band no electronic state exists and also, near the edge of the conduction band very less number of electronic states exist in this energy range. As we go higher as we go above the bottom of the conduction band to higher energies, the allowed electronic states increase significantly ok.

So, this we need to keep in mind . So, this was the scenario for 3D materials, for 3D channel. Now, let us see what happens in a 2D channel and this you might have already guessed that for 2D channel, for a 2D material, the density of state is independent of energy. So, the density of state is a constant function.

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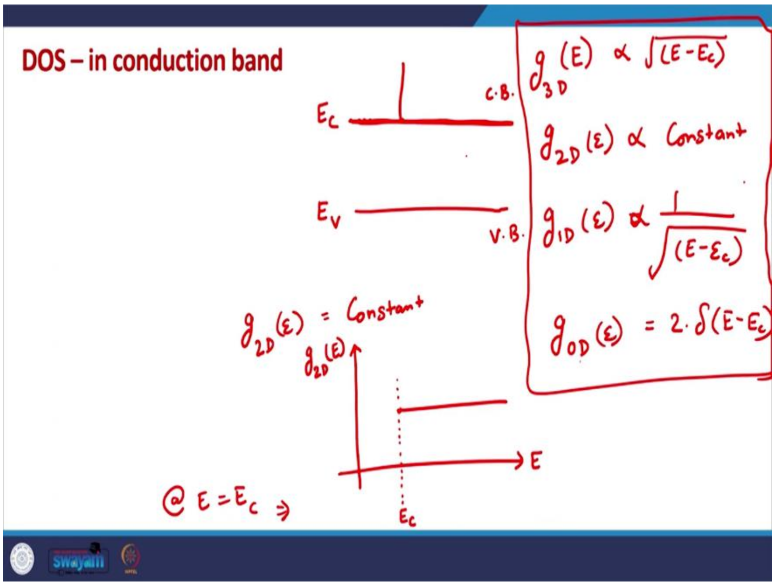

DOS – in conduction band

$g_{3D}(E) \propto \sqrt{(E-E_c)}$

$g_{2D}(\varepsilon) \propto$ Constant

$g_{1D}(\varepsilon) \propto \frac{1}{\sqrt{(E-E_c)}}$

$g_{0D}(\varepsilon) = 2 \cdot \delta(E-E_c)$

$g_{2D}(\varepsilon) =$ Constant

@ $E = E_c \Rightarrow$

So, a 2D density of state in conduction band will be constant. So, if we plot the density of states, it will be a constant function starting from the bottom of the conduction band. It will be a function like this ok. So, what it says is that the number of allowed electronic states in the device is same irrespective of where you are in the conduction band. So, in this entire range the same number of electronic states would be allowed in this entire range.

So, in this case, an electron can exist at the bottom of the conduction band and in fact, it can exist anywhere wherever there is an available state. This is different from a 3D case, where electrons just near to the bottom of the conduction band are very less in numbers because the density of states is very small in that region. Let us see what happens in a 1D case. In a 1D case, the density of states is actually inversely proportional to energy and the situation is exactly opposite to the 3D case.

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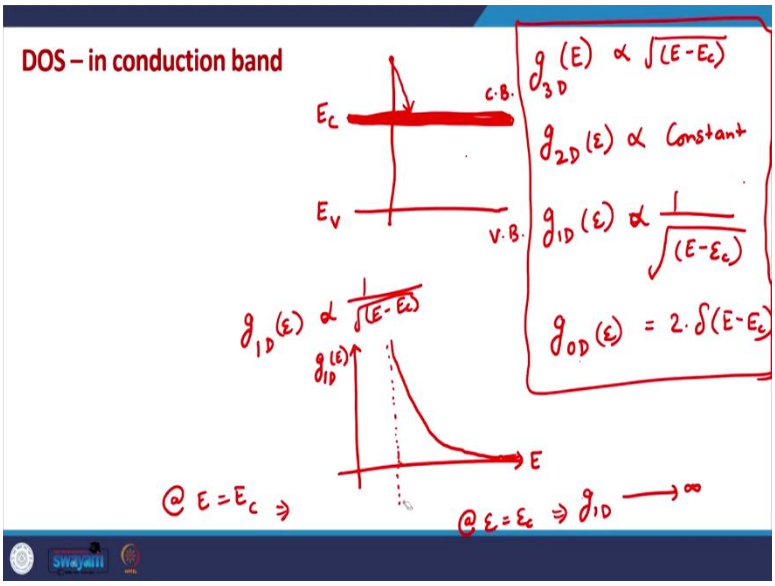

DOS – in conduction band

$g_{3D}(E) \propto \sqrt{(E-E_c)}$

$g_{2D}(\varepsilon) \propto$ Constant

$g_{1D}(\varepsilon) \propto \frac{1}{\sqrt{(E-\varepsilon_c)}}$

$g_{0D}(\varepsilon) = 2\cdot\delta(E-E_c)$

$g_{1D}(\varepsilon) \propto \frac{1}{\sqrt{(E-E_c)}}$

@ $E = E_c \Rightarrow$

@ $\varepsilon = \varepsilon_c \Rightarrow g_{1D} \longrightarrow \infty$

So, in 1D case, it will be inversely proportional to square root of E - Ec. So, this g versus E plot for 1D solids would be like this. Just at the bottom of the conduction band which means at E equals E c, g 1D actually tends to infinity. So, this is the huge number at the bottom of the conduction band.

So, what it means is that at the bottom of the conduction band, an extremely large number of allowed electronic states exist. In fact, most of the electronic states exist at the bottom of the conduction band which means that in 1D solids most of the electrons stay at the bottom of the conduction band.

This is direct to in contrast with 3D solids. So, now, if an electron is excited from the valence band to the conduction band, in most of the cases, it will invariably fall to the bottom of the conduction band because there is huge number of electronic states available there, almost infinite and that is an interesting difference as we change the dimensionality of material or as we change the dimensionality of the channel, such kind of fundamental changes happen in the electronic properties of the material.

So, that is why this kind of analysis, this kind of fundamental analysis is important, if we want to understand the conduction or understand the transport in devices specially in nano devices; where 1D, 2D channels are quite frequent actually. In 0D case, it is just a delta function. So, there are discrete energy levels. It is just like a atomic structure of; even the notion of conduction band and valence band is not very well applicable in 0D materials.

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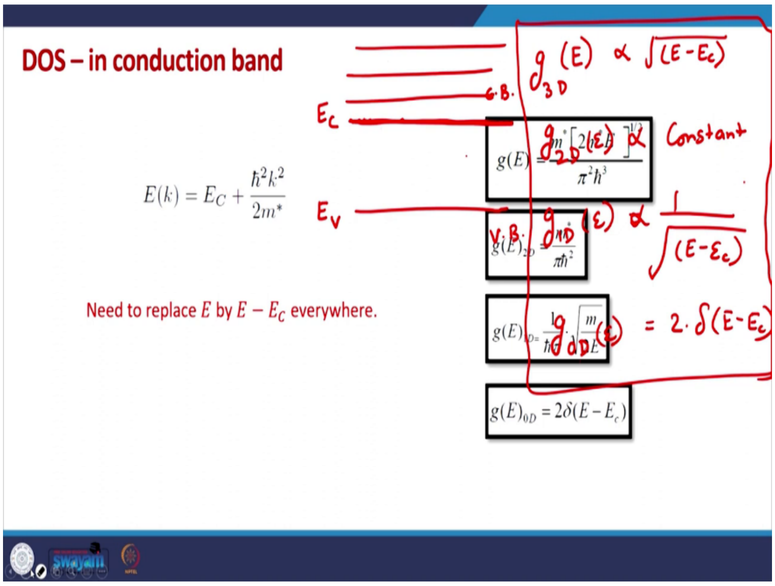

DOS – in conduction band

$$E(k) = E_C + \frac{\hbar^2 k^2}{2m^*}$$

Need to replace E by $E - E_C$ everywhere.

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

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

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

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

So, we will just have allowed electronic states, discrete allowed electronic states, where in each state two electrons can exist ok. So, with this, we essentially conclude our discussion on the density of states.

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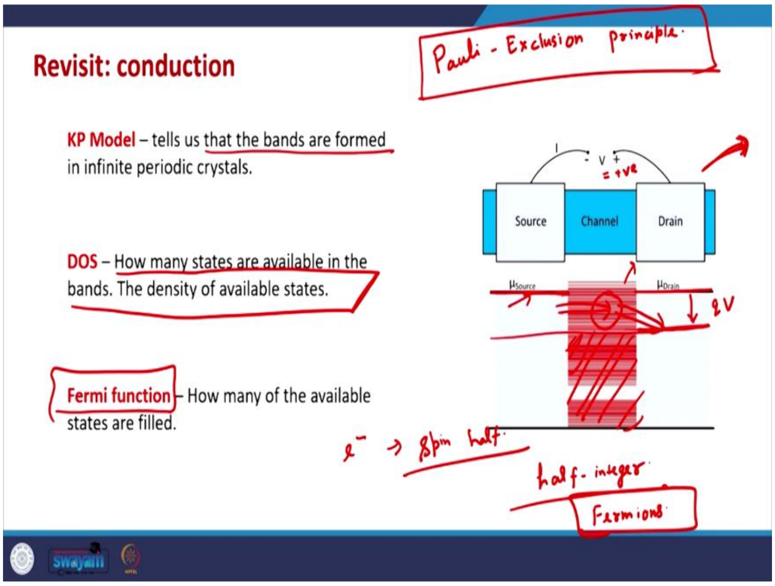

Revisit: conduction

KP Model – tells us that the bands are formed in infinite periodic crystals.

DOS – How many states are available in the bands. The density of available states.

Fermi function – How many of the available states are filled.

The next topic that we are going to discuss is the idea of Fermi function. So, as we have repeatedly seen for conduction, we saw that if this is the 2D device, prototypical 2D device; a two terminal device, not 2D device this is a two terminal device that we take in order to understand the theory of transport and in this two terminal device, if there is no applied voltage, the source Fermi level and the drain Fermi level are at the same level.

If we apply a voltage here, this v becomes positive. The drain Fermi level will go down by a value of q times applied voltage and the source Fermi level will try to fill all the electronic states up to this level. The drain Fermi level will try to fill all electronic states up to this level.

So, all the electronic states below the drain Fermi level will be filled in the channel and these states will be getting electrons from the source and the drain will take out the electrons from these states and this will essentially enable conduction in the device. So, this is the broad idea of conduction.

But before that we sort of need to understand the idea of the Fermi level and the Fermi Dirac distribution function or simply known as Fermi function. So, with the density of states, we could see how many allowed electronic states are available in the solids; especially, in conduction band or even we can also reduce the number of available electronic states in the valence band as well.

Using with KP model, if we go back we saw that mathematically and graphically how bands are formed in periodic crystals. So, now, the last topic that is left before we move on to discuss the idea of conduction or the theory of transport is the Fermi Dirac distribution function.

So, all of us know that electrons are spin half particles and all half integer spin particles, all the particles whose spin is half integer 1/2, 3/2, 5/2, so on; all those particles are known as fermions and on fermions, when a lot of fermions are close to each other, this fundamental principle Pauli’s exclusion principle applies basically.

So, what it means is what this principle says is that no two fermions can have the same quantum numbers; exactly the same quantum numbers. In other words, Pauli’s exclusion principle states that the two electrons cannot occupy the same electronic wave function, when we take spin wave function and the space wave function together ok.

And because of this, if we have a large number of fermions in a system which is generally the case. For example, in solids, we have a huge number of electrons; even in a small channel, we will have a large number of electrons sitting there. Then, because of the Pauli's exclusion principle, they will occupy various states in a certain way.

So, they will follow a certain distribution function which is known as the Fermi Dirac distribution function or simply known as the Fermi function ok. So, the Fermi function that is essentially the idea of the Fermi function and mathematically, this is how it looks like.

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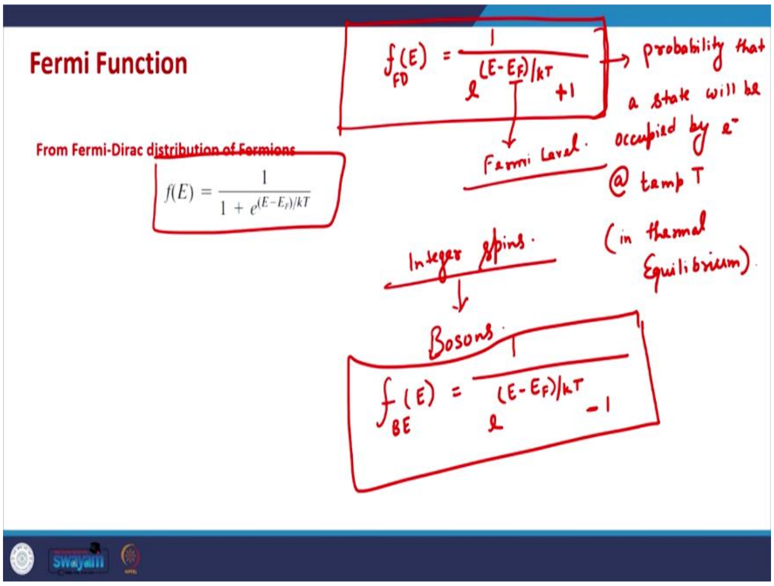

Fermi Function

From Fermi-Dirac distribution of Fermions

$$f(E) = \frac{1}{1 + e^{(E-E_F)/kT}}$$

$$f_{FD}(E) = \frac{1}{e^{(E-E_F)/kT} + 1}$$ → probability that a state will be occupied by e^- @ temp T (in thermal Equilibrium).

E_F → Fermi Level.

Integer spins. → Bosons.

$$f_{BE}(E) = \frac{1}{e^{(E-E_F)/kT} - 1}$$

So, this is a function of energy. This is given as $f_{FD}(E) = \frac{1}{e^{\frac{E-E_F}{kT}}+1}$. This is how the electrons will be distributed in the system. Physically, it corresponds to the probability that a state will be occupied by the electron at temperature T in thermal equilibrium.

So, the Fermi Dirac distribution function physically means the probability that a state is occupied at a given temperature in thermal equilibrium and it depends on E_F which is known as the Fermi level of a of the material.

Now, this is the distribution function of fermions. In nature, there are other particles as well which have integer spins and these particles are known as Bosons essentially and there is no principle like Pauli's exclusion principle for bosons. Bosons can many bosons can occupy the same state, same energy state and the distribution function is known as the Bose Einstein distribution function.

So, let us write this function as BE; f_{BE} and Fermi Dirac as F_{FD} that function is given as. So, these two functions essentially describe how two different kind of particles fermions and bosons are distributed in various energy levels at a given temperature and there is only a small difference and that is the difference of this sign. Here, it is a positive sign in Fermi Dirac distribution; in Bose Einstein distribution, this is the negative sign. But this makes huge difference; this sign makes huge difference in their distribution.

So, we will see how this how Fermi Dirac distribution function is important in our device analysis. We will also see why this probabilistic argument comes about; why can we interpret this as a probability of the state being occupied by electron at a given temperature in the next class.

So, I let you think about this; I will request all of you to think about or go through Fermi Dirac distribution and Bose Einstein distribution function and if you can go through the derivations, at least the theory of these two distributions on your own.

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