Physics of Nanoscale Devices
Prof. Vishvendra Singh Poonia
Department of Electronics and Communication Engineering
Indian Institute of Technology, Roorkee

Lecture - 11
Density of States

Hello everyone. Today, we will discuss the idea of Density of States in more details. We started with this idea in our previous lecture. So, before going into more details of this concept. Let me quickly review what we have discussed so far.

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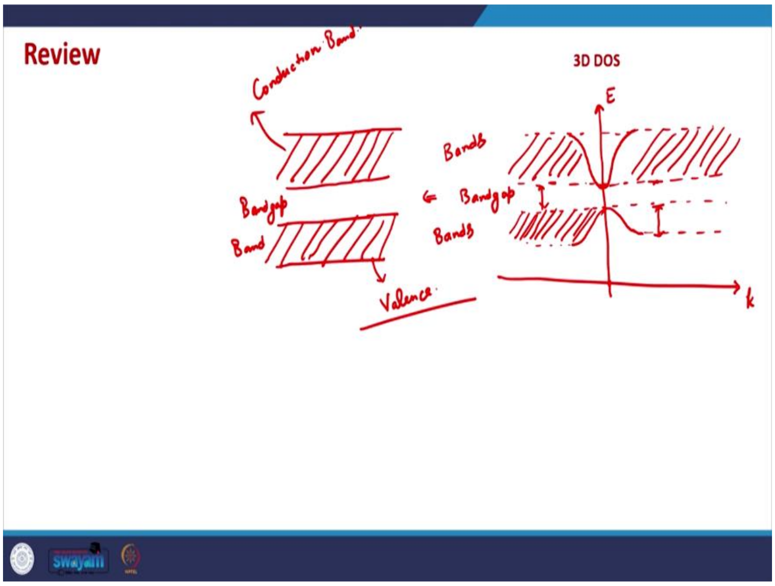
Review

3D DOS

So, what we have seen so far is that because of the periodic potential bands naturally arise in solids, that is the conclusion from the Kronig-Penney model, KP model. And from there we saw that the E k relationship for a 1D solid and which can also be generalized to 2D and 3D solids, but it will be more complicated than the 1D case, this looks something like this.

So, there are; so, we are taking just one portion of the E k plot and this is how it looks like. The E k diagram has energy range, has k values corresponding to certain energy range, and corresponding to other energy ranges the k values are not there, so that is why those energies are forbidden for the electron to take.

Generally, if we have this kind of E k relationship in our band structure, band diagrams, generally, it is represented as something like this. So, this is; so, if we draw lines on the boundaries of allowed E values, then these ranges where, these energy ranges energy values where electrons can be present or electrons can take, these energy values these are known as the electronic bands.

Similarly, this is another electronic band where we have allowed E and k values, which means we have allowed electronic wave functions in these energy ranges. There is this energy range for which no k value exist corresponding to the E values and this is known as the band gaps. This is known as the band gap. And the reason it is known as band gap because there is no allowed electronic wave function in this energy range.

So, generally, this is plotted as like this, in our standard representation of energy bands this is how we plot the energy bands. This you might have already seen in band diagrams of semiconductors and electronic devices. This is the band and this is the band gap. And like this we have various bands and various band gaps in a semiconductor, or generally in a solid typically in metals we, metals also we have many bands, but in metals what happens is generally two bands are overlapping.

So, in, so that is why there is no energy value for which k does not exist, which means electrons can occupy all energy states in metals, ok. But semiconductor, we will talk about semiconductor, mostly semiconductors in this course. So, that is why we will be more concerned about the electronic properties in semiconductors and this is the situation in semiconductors.

The highest occupied band is known as the valence band. So, there are various such bands, among them the highest occupied band is known as the valence band and the lowest unoccupied band is known as the conduction band. And briefly they are written as VB and CB. So, the highest occupied band is valence band and the lowest unoccupied band is the conduction band.

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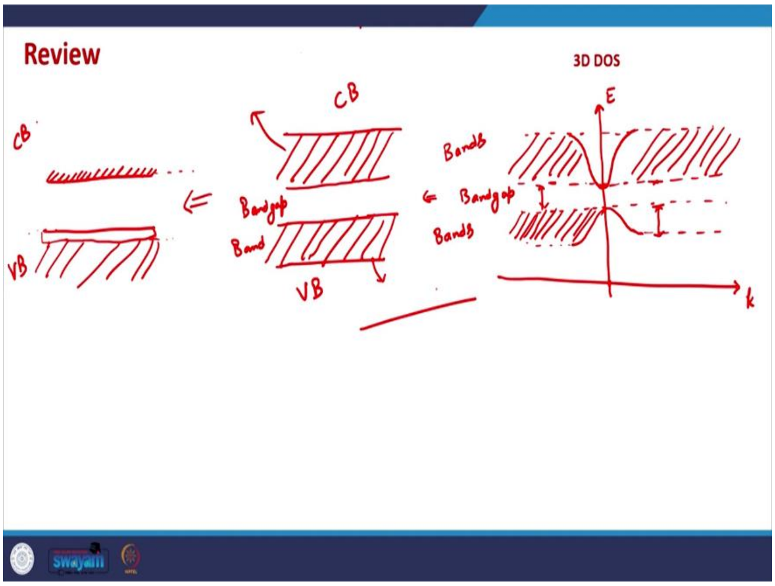

Review

3D DOS

And generally, we just plot the top of the valence band and bottom of the conduction band because in valence band most of the electronic states are filled apart from some states near the top of the valence band.

So, most of the states; so, if this is the valence band this is the conduction band, most of the electronic states are filled which means electrons exist, for most of the energy values up to this value, but only certain energy values, only a small number of states or a small range of energy values where electrons do not exist which means that those electronic states are empty.

So, that is why we generally plot just the top of the valence band and bottom of the conduction band because in conduction band most of the electronic states are empty, only some states near the bottom of the conduction band are filled. So, generally, at room temperature or at our operating temperatures, some of the electrons gain enough energy, so that they can make a jump from the valence band to the conduction band and they go from the top of the valence band to the bottom of the conduction band.

So, that is why in our band diagrams and band structures, we mostly plot the top of the valence band and the bottom of the conduction band. And in between we have a band gap and that is where most of the semiconductor physics takes place, that is the most important sort of regime for to deduce electronic properties of semiconductors.

So, this is about the solids, this is in other words we have already discussed that from here we also saw that generally in a device the electron does not have a definite energy and a definite momentum value, so that is why the electron in a device or electron in a small region cannot be described by a single wave function.

So, that is why we need to take a bunch of wave functions many wave functions corresponding to different energy values and that becomes a wave packet and that is what actually describes the electron. And from the notion of the wave packet comes the idea of effective mass.

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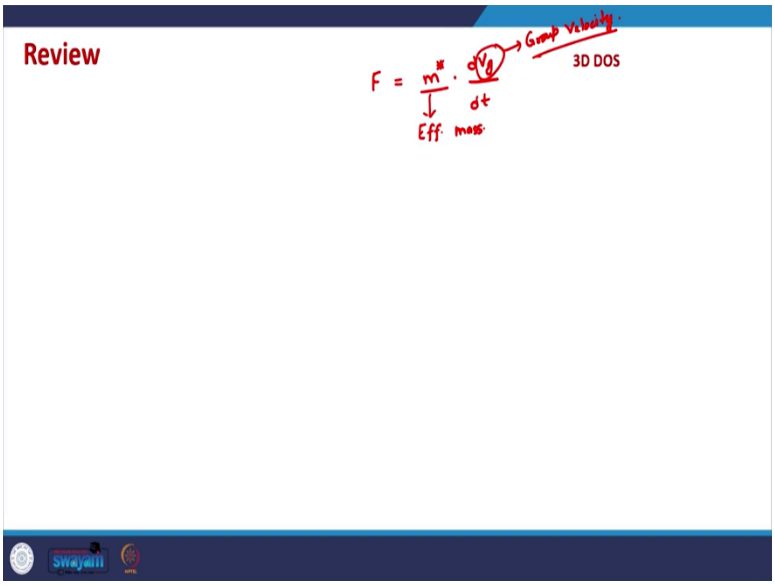

Review

$$F = \underset{\substack{\downarrow \\ \text{Eff. mass.}}}{m^*} \cdot \frac{d\,\boxed{v_g} \rightarrow \text{Group Velocity.}}{dt}$$

3D DOS

So, when electron is described by a wave packet, then an external force acting on the electron can be described as F=$m^* \frac{dv_g}{dt}$, where m^* is the effective mass and v_g is the group velocity of electronic wave packet, and $\frac{dv_g}{dt}$ is in a way acceleration of the wave packet.

So, this equation looks pretty much similar to a classical equation of motion or Newtons Second Law of motion and that makes our analysis of devices very easy. Now, we will see, now we are gradually coming towards actual analysis of devices.

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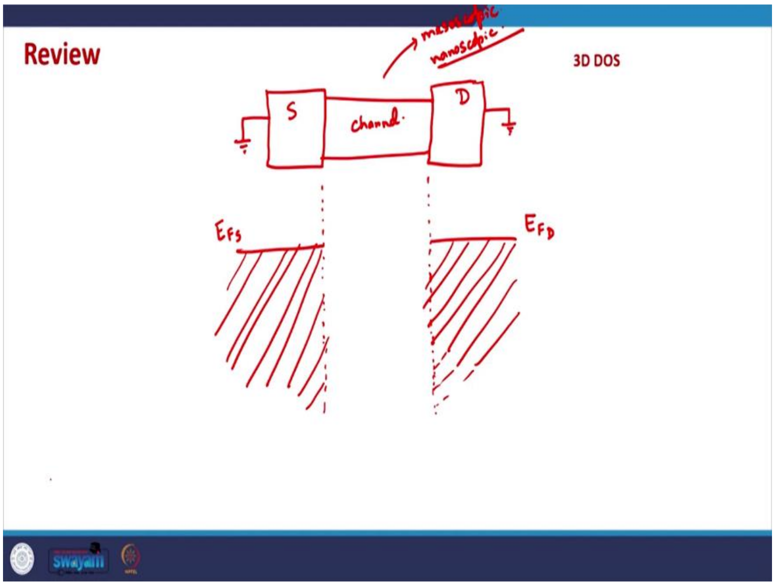

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3D DOS

So, as usual we start with a two terminal device and a two terminal device looks like this. So, we have a channel region in between and on the left side we have the so called source contact, on the right side we have the drain contact. In this diagram, the channel region is shown as larger than the source and the drain, but that is not the case. Here it is drawn like this just for sake of representation, sake of understanding, so that we can understand things properly.

Generally, channel region is very small it is mesoscopic channel. Mesoscopic means not macroscopic, not entirely nanoscopic, it is in between few times of nanometers on nowadays even a nanoscopic channel nanometers few nanometers length, source and drain regions are relatively large as compared to the channel region.

And the conduction takes place in this way, source and drain regions are typically metallic bulk. So, that is why their electronic distribution can entirely be defined by their Fermi level. We will come to this idea in a little bit after this idea of density of states. But there is an energy level which governs the distribution of electrons in any solid, specially in bulk solids in equilibrium, and that is known as the Fermi level.

In metals all the electronic states, below Fermi level are filled. So, all the states below Fermi level are filled like this. And in the channel region, there are certain energy states that are present. So, when we do not have any applied voltage which means both source and drain terminals are at the same voltage which means we can consider both source and drain to be grounded, in that case both Fermi levels are at the same level, so no conduction happens in the device, ok.

So, that is everybody is in equilibrium, no conduction is taking place, and no electron is flowing through the device. So, the equilibrium just to sort of let me take a moment and explain what is equilibrium. Equilibrium is used many times in not only in electronic systems, in almost all the systems. So, equilibrium is the state of systems where each and every process happens, so each and every process has a corresponding counter process.

So, for example, in equilibrium, if electron, if n number of electrons are flowing from left to right, it means that we will say that this system is in equilibrium when the same number of electrons will be flowing from right to left with exactly same velocity, same kind of situation same kind of parameters.

So, every process is countered by the equal and opposite process. So, that is that state of the system is known as the state of equilibrium. So, this is the equilibrium when no voltage is applied, everybody is the every level is at the same; these two Fermi levels are at the same energy level.

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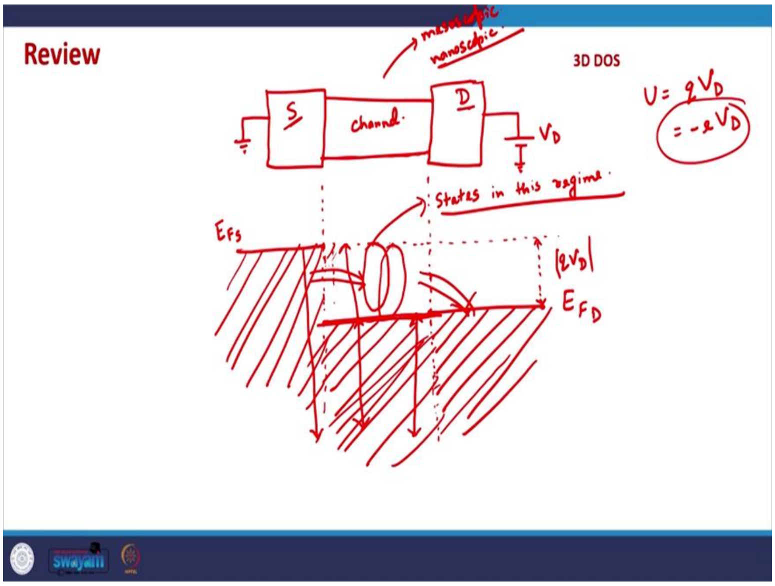
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3D DOS

But when we apply a small voltage on the device which means we apply a positive voltage, generally that is the convention on the drain terminal, a positive voltage will mean that the electronic potential energy will go down by minus e times V_D, where V_D is the applied voltage. So, which means that the drain Fermi level will go down by this value.

So, now, the situation becomes something like this. The source Fermi level does not change because it was grounded before and it is grounded even now, but now the drain Fermi level goes down by a value of q times V_D.

So, now the drain Fermi level has come down by this value. So, this is the position of drain Fermi level before we applied any voltage, now it has gone down by q times V_D value. This is the magnitude of the decrease in the level of the drain Fermi level, ok.

Now, in devices and by definition, all electronic states below Fermi level are occupied at T equal to 0 kelvin and as temperature increases some of those states become empty. But, generally in metals it is considered that all the electronic states below Fermi level are filled. And when we put such material in contact with the channel, like in this device, in this device we have put two such contacts, in two such material source and drain materials in contact with the channel.

Now, what happens is when we put the source terminal in contact with the channel, what it tries to do is it tries to fill all electronic states below source Fermi level in the channel. So, what it tries to do is, it tries to fill all these electronic states below the source Fermi level, so just to maintain the equilibrium that is the scenario, that is basically the job of the Fermi level as well.

And here we are considering that the source terminal and also the drain terminal are extremely large as compared to the channel region, and even if we take out some electrons from the source or from the drain, it does not change the Fermi level. Although, it can change, in principle it can change, it depends on the number of particles or number of electrons in the material, the Fermi level depends on that and we will see that a little bit later.

But here we are assuming that the source and the drain terminals have a large number of electrons, and even if some electrons go from the source to the channel the levels do not change. So, now, what happens is the source Fermi level is trying to fill all electronic states in the channel up to this level, all electronic states in this range are being trying to filled by the source contact. And the drain contact is trying to fill all electronic states in the channel up to this level ok, similarly.

So, what it implies is the electronic states up to this level are being tried by both source and drain terminal. They are trying to fill these electronic states, both of these contacts are trying to fill these electronic states. And since, the number of electrons in the source region and in the drain region are extremely large, they will actually fill all the electronic states below this level, which is basically the drain forbidden.

But the states in between E_{FS} and E_{FD}, the source Fermi level and the drain Fermi level, the source terminal is trying to fill them, but the drain terminal will try to empty them. Drain terminal will try to extract the electrons from the channel in this range because it will try to make sure that only states up to this level are filled.

So, there is a sort of competition between the source terminal and the drain terminal in which the source is trying to fill the states, the drain is trying to drain out electrons from them, and that is how the conduction takes place, ok.

So, that is why the number of states in channel in this region is extremely important. Electronic states in this regime is extremely important. For example, if the channel has, channel material is such that there is no electronic state in the channel in these between these energy values, in that case no conduction will take place in the channel whatever be the voltage that we apply on the drain terminal, ok.

So, if there is no state in the channel between the source Fermi level and the drain Fermi level, the conduction cannot take place. So, the conduction does not happen just because we apply a certain voltage, specially in and that is specially true in mesoscopic or nanoscopic devices.

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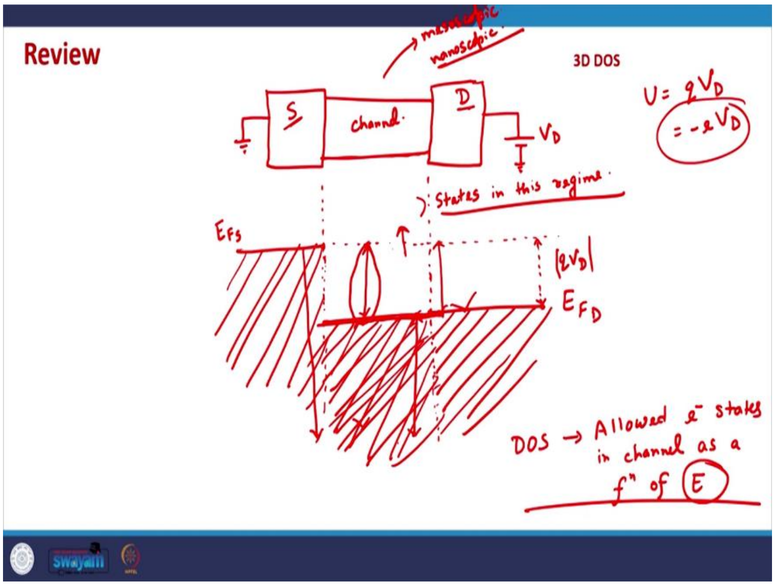

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3D DOS

In addition to an applied voltage, we need electronic states in this region, the region between the source Fermi level and the drain Fermi level. We need allowed electronic states in this region. If the electron, if the channel has a band gap in this regime no conduction will take place whatever be the applied voltage, because even if the source is trying to fill all the electronic states here, but there is no electronic state here.

So, you can it cannot fill any electronic state. And no electron can shift from source to channel to drain. That is why the number of the number of electronic states in the channel is an important idea, very important idea, because in order to understand the conduction in devices or in materials, apart from the applied voltage we need allowed electronic states in this regime, the regime between the source Fermi level and the drain Fermi level.

And that is why we are trying to understand the idea of the density of states, because the density of states tells us about the allowed electronic states in channel as a function of energy. So, we will be able to know how many electronic states exist as a function of energy in the channel.

Apart from conduction in order to see how many electrons are there in the channel or what is the steady state number of electronic states electrons in the channel, we also need to know how many states are there even in this regime.

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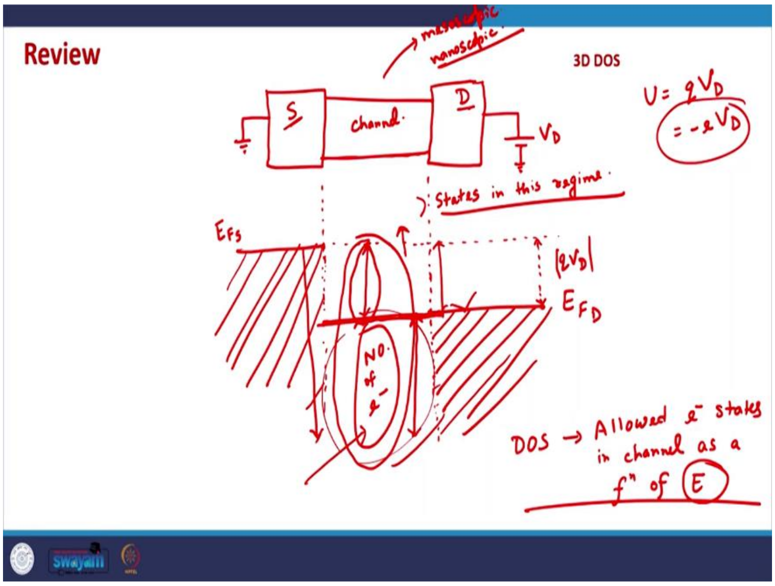

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3D DOS

So, even in this regime, even in this regime, we need to know electronic states because it will tell us about the number of charge carriers in the channel which means how much charge the channel is holding while it is doing conduction. Because all these electronic states are filled, which means electrons exist in all these states.

Even if they were not there earlier, before contacting the channel with source and drain even if these states were empty, but now after contacting the source and the drain to the channel these states will be filled which means a certain charge will be there in the channel which will not move, ok.

That will tell us about the charge concentration or the number of electrons in the device or in the channel. And that will also govern, that will also play some role in electrostatics of the device, ok.

So, that is why it is very important to know how many states are there how many allowed electronic states are there as a function of energy. So, that we can understand the idea of conduction, the idea of transport in devices well.

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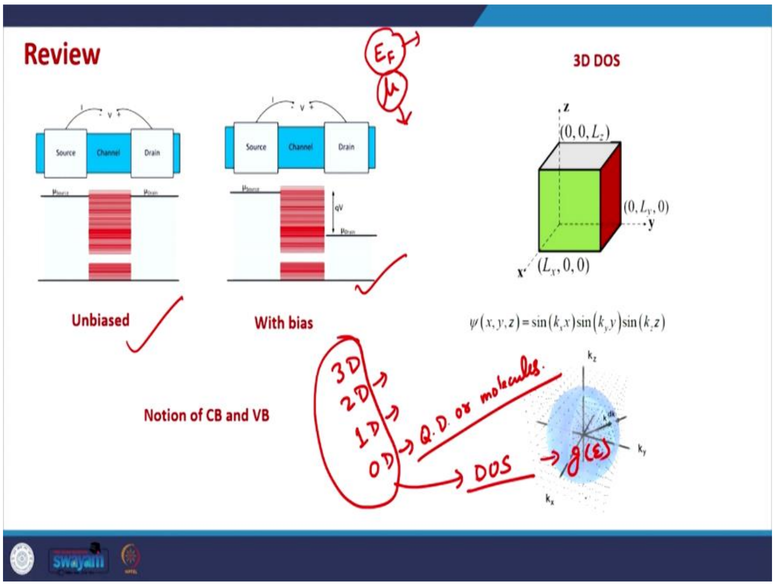

Review

Unbiased

With bias

Notion of CB and VB

3D DOS

$\psi(x,y,z)=\sin(k_x x)\sin(k_y y)\sin(k_z z)$

And that is what we were we started with in our, also in our previous class. We saw that this we have seen unbiased two terminal device looks like this. With bias, the source and drain Fermi levels change. Fermi level, just a short note Fermi level is represented as E F or mu. Generally, this notation is used mostly by physical chemists, people in chemistry. This notation is mostly used by solid state physicists, ok.

And this channel region can be a 3D channel, like most of our conventional devices. This can also be a 2D channel, like graphene nano ribbon or even MoS 2 material. This can be a 1D channel, like a nano wire or this can be a 0D channel. For example, quantum dots or molecules.

So, we need to understand how many electronic states would exist in these channels as a function of energy and that is essentially what we obtain from the density of states. So, density of states is represented as g(E) and that is what we will be calculating.

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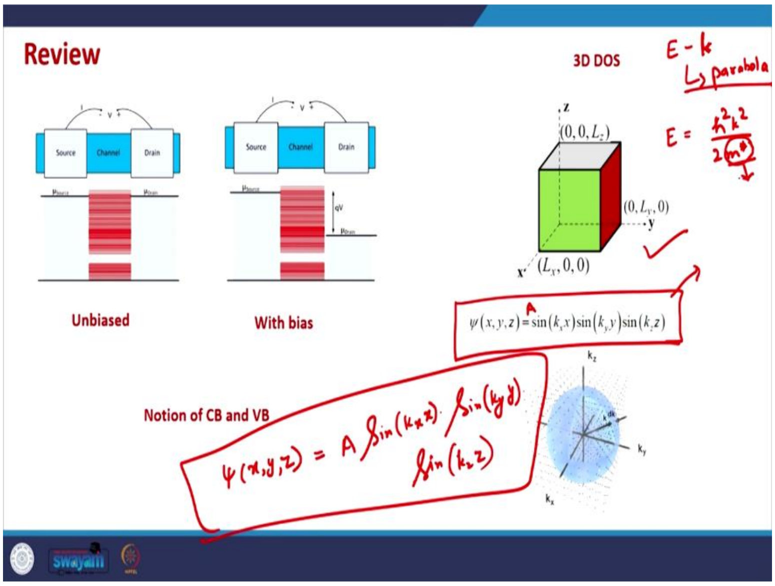

Review

3D DOS

$E - k$

$\hookrightarrow$ parabola

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

$\psi(x,y,z) \overset{A}{=} \sin(k_x x)\sin(k_y y)\sin(k_z z)$

Notion of CB and VB

$\psi(x,y,z) = A \sin(k_x x) \cdot \sin(k_y y) \sin(k_z z)$

So, we started our discussion with density of states in a 3D material, 3D channel. And this is how a 3D channel looks like. It is extended essentially in all 3 directions, Lx in x direction, Ly in y direction, Lz in z direction. And from the generalization of the solution of particle in a box situation, the wave function can now be written as, the electronic wave function can now be written as $\Psi(x, y, z)$ can be written as a constant times sin $k_x x$ into sin $k_y y$ into sin $k_z z$.

Here there are certain underlying assumptions, so the 3D solid will have various lattice points in the solid. So, there will be many lattice points in the solid. So, because of that there will be a crystalline potential. Apart from that electrons will be interacting with the, electrons will have, various electrons flowing in this 3D material will be interacting with that crystalline potential.

But as we saw that if the E k diagram, the E k relationship if it can be approximated by a parabola, then the idea of effective mass is applicable. And in that case, if we can write down the E k relationship like this, $E=\frac{\hbar^2 k^2}{2m^*}$, in that case we can assume that this 3D solid is like a big potential well in 3 directions. And all lattice points effect can be considered by this effective mass. The effect of all the lattice points is now captured by the effective mass, ok.

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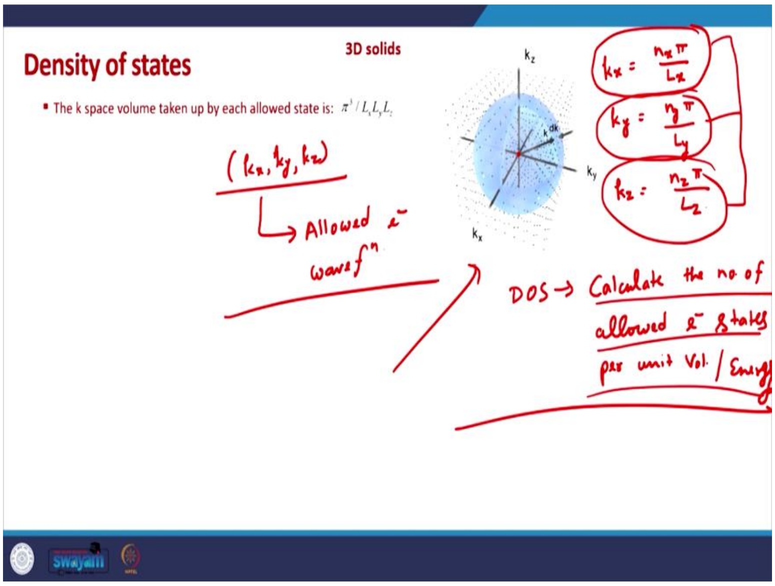

Density of states

3D solids

- The k space volume taken up by each allowed state is: $\pi^3 / L_x L_y L_z$

(k_x, k_y, k_z) → Allowed e^- wave f^n

$k_x = \frac{n_x \pi}{L_x}$

$k_y = \frac{n_y \pi}{L_y}$

$k_z = \frac{n_z \pi}{L_z}$

DOS → Calculate the no. of allowed e^- states per unit Vol. / Energy

So, once we realize that the electronic wave functions in a 3D solid is a direct generalization of electronic wave function in a 1D solid, now there are allowed k values. So, the allowed k values will be like a 1D solid. These allowed k values will be k_x equals $n_x\pi/L_x$, k_y equals $n_y\pi/L_y$, and k_z equals $n_z\pi/L_z$, ok.

And the idea of density of states is to basically calculate the number of allowed electronic states per unit volume as a function of energy. So, that is the idea of density of states. So, essentially, we need to calculate the number of allowed electronic states in the device.

In order to do that, as you can see from here an allowed combination of k_x, k_y, k_z, this combination gives us an allowed electronic wave function, ok. So, all allowed combinations of k_x, k_y, k_z which can be deduced from these 3 relationships, these will give us various electronic wave functions which the electron can take in a 3D solid. And, so these k points combination of these k points will correspond to the allowed electronic states in solid.

So, if we need to calculate the number of allowed electronic states in the solid, we just need to calculate the allowed k points in the solid. So, that is why we move to the k plane. k plane means, now, we plot k_x, k_y, k_z axis and we plot the allowed k points in k on k_x, k_y, k_z axis.

And here as you can see from this plot, all these points are the allowed electronic states, ok. So, migrating from a real plane, from a real space to k space makes the counting of electronic states easier, so that is why we do that. Because this sometimes becomes confusing why we are dealing in the k space, and that is just to calculate the allowed number of electronic states because it can be done straight forwardly in k plane.

So, that is what we will do in our next discussion. We will actually calculate the number of allowed k points and from there we will deduce the density of states for 3D solids, then we will move on to 2D solids, then 1D solids, then 0D solids, and then we will discuss how this idea of density of states is applicable in electronic devices.

Thank you for your attention. I will see you in the next lecture.

Thank you.