Physics of Nanoscale Devices
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Lecture - 10
Density of States

Hello, everyone. Today, we will discuss the idea of Density of States in devices; electronic devices. Let me quickly review what we have discussed in last couple of classes. We discussed how the bands arise naturally in solids when we solve Schrodinger equation for electrons in solids and that was done using K P model ok.

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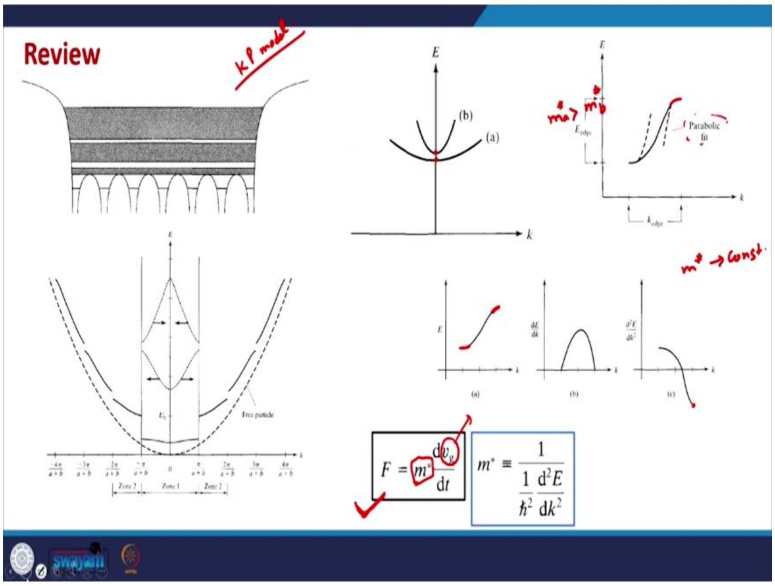

With this idea we could see that we can have an equation of motion or equation of action so to say. When we consider electrons in devices as wave packets the equation of action looks exactly like Newton's second law of motion, where the mass is replaced by the effective mass the so called effective mass and the velocity of the particle is replaced by the group velocity of electronic wave packet.

And there are some interesting implications of this equation of action. We can see that even if electrons have same energy two electrons, but they are in different bands and the curvature of the bands are different in that case the effective mass of electrons would be different, effective mass of electron in a would be more than effective mass of electron in b.

So, in band a, the electron behave like a heavy particle and in band b, it will behave like a light particle. Apart from that another interesting conclusion was that at the bottom of the bands the curvature is positive. So, the electron behave like a positive mass classical particle, but at the top of the bands the curvature of E k plot is negative and electrons behave as if their mass is negative, they behave opposite to what a classical particle will behave ok.

Apart from this we also saw that there are certain constraints in which this equation of action can be used in our analysis and that is true, when the E k plot can be approximated by a parabola. So, in for those E and k values, where the E k plot takes a parabolic kind of fit where the E k plot can be fit by a parabola there the effective mass would be constant it would not be dependent on energy and there we can directly use this equation of action ok.

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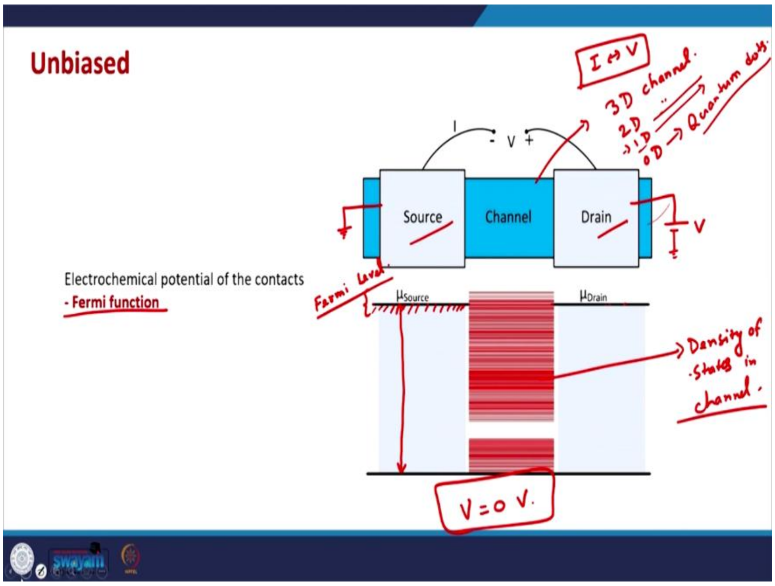

So, with this we moved on to a second idea. And we come back now to a two terminal device in which we have a source we have a drain and we have a channel region. In this two terminal device, generally the source terminal is grounded the drain terminal is applied with voltage V and the source and the drain are bulk material and the channel region is a small mesoscopic or nanoscopic region of semiconductor let us say.

The electronic constant. So, in order to sort of understand the I-V characteristics which is the most important thing that we would like to know about a device how much current would flow through the device when we apply a certain voltage. So, the I-V characteristics is ultimately what we want to calculate or deduce from our analysis. In order to understand the I-V relationship or how much current would flow through the device we first need to understand how many electrons are there and how they are distributed in the system.

So, then only we can sort of extend that idea to how many electrons will flow through the device. So, in bulk materials the concentration of electrons or the number of electrons at a certain energy at a given temperature is calculated by a function called Fermi function and there is an idea or there is a concept called Fermi level or in other words electrochemical potential of the material.

So, the Fermi level is the level up to which all the electronic states all the allowed electronic states in the system are filled at T equal to 0 Kelvin. So, at absolute zero temperatures, the level up to which all electronic states are filled is known as the Fermi level of the material and this idea this is a statistical idea. So, that is why it is well defined in bulk materials, but sometimes it is also used in nanoscale or mesoscopic devices as well.

So, by defining the Fermi level and Fermi function for source and drains we can see and these two materials are metals. So, the electrons are there are lots of electrons all. So, it has the as you might know that metals have bands overlapping bands. So, all the electronic states up to Fermi level are assumed to be filled in metals. So, in source and drain contacts all the electronic states below Fermi level are filled generally at T equal to 0 temperature above T equal to 0 temperature some of these electrons can go at higher energy states as well.

And the source and the drain these contacts they will have a continuum of states below the Fermi level and even above the Fermi level because these are the bulk material. And so, that is why allowed electronic states will be a continuum of states. So, almost at all possible energies electrons can exist because they are metals and they are bulk materials.

So, for source and drain contacts just by knowing their Fermi level and Fermi function at non zero temperatures we can figure out the distribution of electrons how many electrons exist at what energy this we can easily deduce. But for channel region which is a small region in modern devices electrons do not take may not take actually may not take continuum of energy values.

So, there may be some energies which might be disallowed because this is a semiconductor. So, there might be a band gap moreover this is a small region and confinement as we saw the confinement creates discretization. So, the electronic states or the energy levels might be discrete. So, in order to understand how many electronic states exist in channels or how many electrons can channel sort of contain we need to understand this idea of density of states in the channel ok.

So, this is what we are going to discuss from this class onwards also this channel in modern devices this can be a 3D channel 3 dimensional channel, it can also be a 2D channel, it can be a 1D channel, it can as well be a 0D channel. By 3D channel; we mean a semiconductor which is basically a channel which is which has dimensions which extends in all three directions.

A 2D channel by 2D channel we mean that it is like a graphene nanoribbon. The dimension in the third direction or the length in the third in one direction is extremely small as compared to its dimension in other two directions. So, it has the length or the extent in one dimension is very small as compared to the extent in other two dimensions. A 1D channel can be a nano wire whose extent in two dimensions is very small as compared to it is extent in third dimension.

And a 0D channel means by a 0D channel we mean that its extent in all three dimensions is very small like molecules or quantum dots. So, in modern day devices this channel can be a 3D channel a 2D channel 1D channel or 0D channel. So, we need to understand the density of states in all these kind of channels and once we are equipped with this understanding we will be in a position to sort of understand the transport of electrons in the devices.

Because we would and apart from that apart from density of states we will also need to know about the Fermi function; once we understand these two ideas we will be in a position to understand the transport and I-V characteristics of the device ok. So, this is an unbiased device unbiased by unbiased means we mean V the applied voltage V is 0 volts.

So, at 0 volts the source electrochemical potential the source Fermi level and the drain Fermi level would be at the same level because they are the same material no voltage applied they are at the same temperature. So, their Fermi level will be the same.

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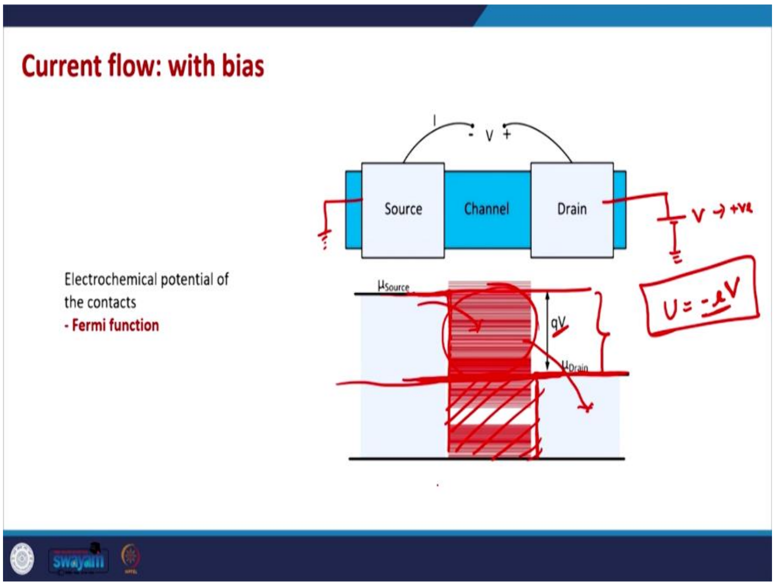

But when we apply a bias, so for example, if we apply a positive voltage on the drain terminal this becomes a positive voltage the source is grounded. By virtue of the positive voltage the potential energy of electrons will go down in the drain terminal because the potential energy is given as the electronic charge which is essentially minus e where e is the unit charge times the applied voltage.

And since the potential energy goes down the electrochemical potential or the Fermi level will also go down by this value q times V where q is also the unit charge ok. So, now with application of a voltage what happens is that the source Fermi level is now higher than the drain Fermi level ok and there are certain electronic states in the channel.

So, now, what happens in this device is that the source contact tries to fill all electronic states in the channel adjacent to the source up to its Fermi level. So, the source tries to fill electronic states up to this level ok and the drain terminal where the Fermi level is now lower than the source Fermi level it tries to fill electronic states up to its mu drain its Fermi level.

So, there is now a competition between the source terminal and the drain terminal. The source is trying to fill all electronic states up to this energy and the drain is trying to fill all electronic states up to this energy. So, all the electronic states which are common to both of them which means all electronic states in the channel in this region will now be filled because both source and drain are trying to fill these electronic states.

But the electronic states which lie between the source Fermi level and the drain Fermi level which means these electronic states in the channel these electronic states the source is trying to fill them with electrons. Because it has enough number of electrons and its Fermi level does not change with flow of few electrons into that channel the drain is trying to fill to make sure that only electronic states up to this level are filled. So, which means that the drain terminal is now trying to make these states empty of the electrons.

So, the source is pumping electrons in these electronic states and the drain is pulling out electrons from these energy states and that is how the conduction basically takes place in a device, in a two terminal device ok. So, this is what we will understand, but before going into more details of this let us begin with the idea of density of states.

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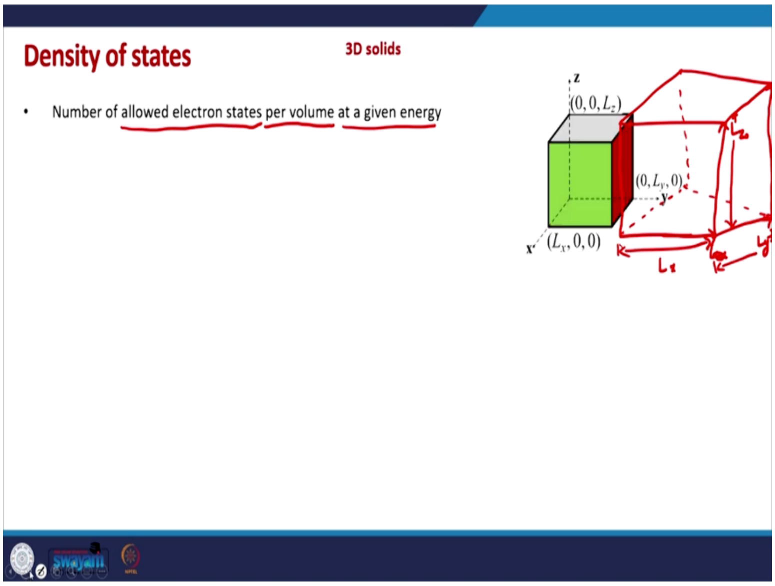

Density of states in very simple terms is; the number of allowed electronic states number of allowed electronic states in a material per unit volume of that material at a given energy. So, at a given energy number of electronic states valid electronic states per unit volume in a material this is the simple definition of the density of states in any material or in a solid state devices. And as we discussed the channel can be a 3D channel, a 2D channel 1D channel or even a 0D channel.

So, let us see how the density of states will look like in a 3D channel. So, let us take a 3D material and what do we mean by a 3D material? A 3D material, a 3D channel by a 3D channel; we mean that the channel will have certain length, certain width and certain height. So, that so this is a 3D material that can be used as a channel. It has let us say L_x length L_y width and L_z height ok. So, this is L_z this is L_x this is L_y.

And in order to make a device out of this material we just need to put contacts at two points of this and then we are basically we will have a two terminal device. And but in order to understand the electronic transport or the electronic distribution we need to see how many states, how many electronic states would be allowed in this particular material.

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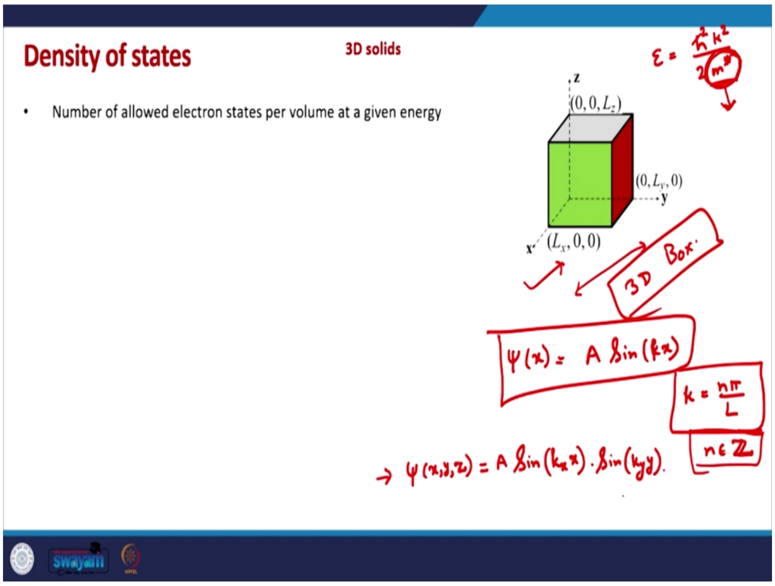

So, this is a typical 3D solid on x y z axis it has L_x extent on x axis, L_y on y axis and L_z on z axis. And if we assume if you make a simple assumption that for all energy values or for the energy values at which we are interested which means at the bottom of bands and the top of the bands; generally these are two regimes of E k plot where we are most interested in because that is where the entire sort of electron and hole transport takes place.

So, in these two regimes this E k relationship is parabolic let us say and the so, that is why the mass of the electron now needs to be taken as the effective mass that we studied in the previous classes. So, let us assume that that in the regimes of interest the E k plot is like a parabolic plot which is not a bad assumption I would say which is true in most of the cases, but instead of regular mass of electron we need to take the effective mass of electrons.

So, the E k plot will look like E would be $\frac{\hbar^2 k^2}{2m^*}$ and now with this notion of effective mass we can sort of ignore all the crystalline potential and the quantum mechanical nature of the electrons. Or, in other words the effect of crystalline potential and the quantum mechanical nature of electrons is now encapsulated in the idea of the effective mass ok.

So, with by assuming electron to be a particle with effective mass this 3D solid can be considered like a 3D box we can ignore the or sort of we can do away with the crystalline potential and the quantum mechanical nature or the quantum mechanical interaction of electrons with the crystal with the atomic course. So, now electron is just a particle in a 3D box like situation in this 3D solid.

So, in order to calculate the density of states how many states would electronic states would exist at a given energy we need to see or we need to sort of solve again we need to start with the solution of the Schrodinger equation in this case and this kind of solution we have already done.

We have already solved Schrodinger equation for a particle in a 1D box where the electron is confined in a one dimensional box. Now, it is just a generalization of the 1D box situation it is now a 3D box and in this case the solution will be a natural generalization of the solution of the particle in a 1D case.

So, if you recall the wave function for particle in a 1D box was A sin (kx), where k was k could take these values of n was integer any integer ok. So, the wave function of electrons in a 1D box was A sin (kx) where k could take values like n$\pi/$L where L was the length of the box and n could be any integer. Now, in a 3D box, I am directly generalizing this solution the electronic wave function would be $\Psi(x, y, z)$ in 3D case it would be a constant times sin k_xx sin k_yy times sin k_zz.

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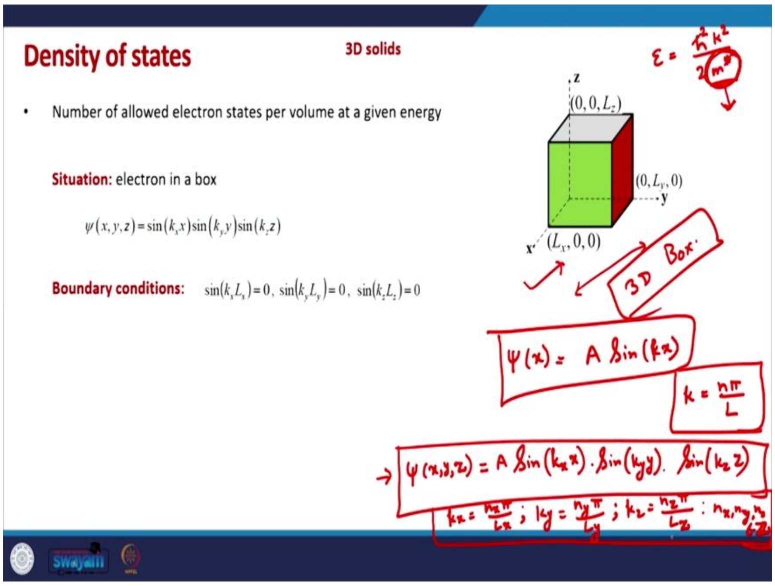

So, this is the electronic wave function in a 3D box when the electron is confined entirely in the 3D box where now k_x is $n_x\pi/L_x$, k_y is $n_y\pi/L_y$ and k_z is $n_z\pi/L_z$ where k_x is n_x n_y n_z are integers set of they can be any integer from the set of integers ok. Now, we need to see how many electronic states would exist at a given energy we need to sort of visualize or we need to calculate we need to count the number of electronic states at a given energy that is what we need to do.

In order to do that calculation it is always easy. So, since as you might have already seen from the solution of the wave function different wave functions exist for a for different values of k's k_x k_y k_z. So, in order to calculate the number of electronic states or in order to calculate the number of allowed electronic wave functions we need to calculate different k values in the system basically.

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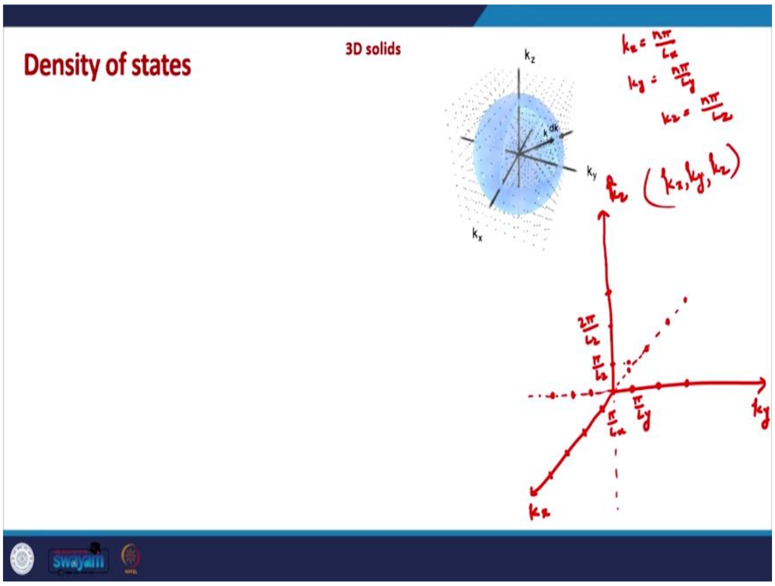

So, that is why we plot the solution k points on the in the k plane which means we have k_x, k_y, k_z axis sorry we have k_x, k_y, k_z axis and the allowed k values $n\pi/L_x$, $n\pi/L_y$ and $n\pi/L_z$ ok. So, on the k axis in the allowed values will be π/L_x, $-\pi/L_x$, $2\pi/L_x$, $-2\pi/L_x$, $3\pi/L_x$, $-3\pi/L_x$ and so on basically.

Similarly, the allowed k_y values are π/L_y, $-\pi/L_y$, $2\pi/L_y$, $-2\pi/L_y$, $3\pi/L_y$, $-3\pi/L_y$…Similarly the allowed k_z values are if we plot on k_z axis these are π/L_z, $-\pi/L_z$, $2\pi/L_z$, $-2\pi/L_z$ and so on and apart from these axis points there can be any point in the plane in this 3D plane. Basically, any combination of k_x, k_y, k_z any combination of allowed k_x, k_y, k_z would be a valid solution for Schrodinger equation.

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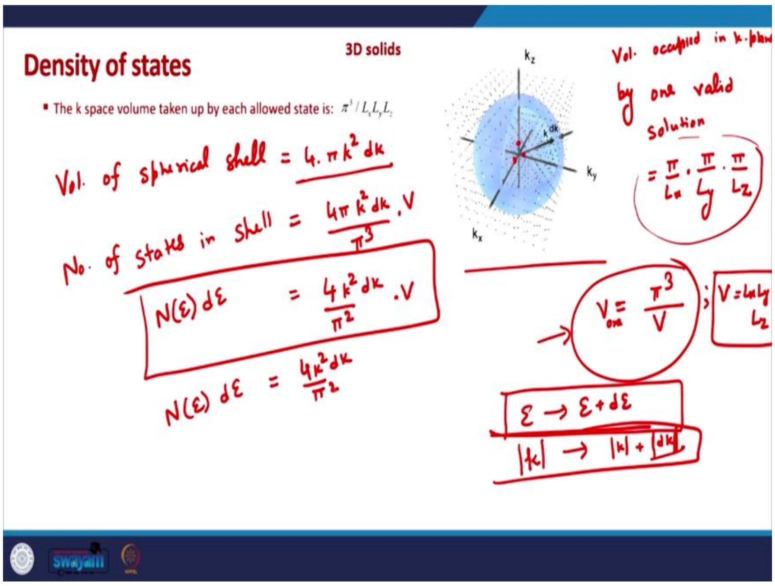

So, this plot basically does that it plot all possible all allowed k points in the k planes and these are the discrete points in this three dimensional k plane. And by their discreteness or by visualizing the allowed solutions in k space we can sort of visualize or we can sort of count the allowed number of electronic wave functions in the system.

So, now from the solution of Schrodinger equation we deduced or we find out the allowed k points and we plot the allowed k points in the k plane 3D k plane. And now, we will need to count the distinct solutions of electronic wave function and then we would need to divide that by the volume of the solid in order to calculate the density of states.

So, that is the sequence of calculating the density of states in any system. So, in this k plane if you closely look the volume occupied in k plane by one valid solution or by each allowed state is π/L_x times π/L_y times π/L_z. So, this is the volume of a single electronic allowed electronic state in the k plane. This is the volume of one state one allowed electronic state in the $\frac{\pi^3}{V}$ where V is the L_x L_y times L_z volume of the solid in physical plane. So, this is the volume of one allowed state in k plane 3D k plane ok.

Now, in order to see how many k states would exist from energy E to energy E plus d E. We need to see how many electronic states exist from a k value certain k point to k + dk and to calculate this number we plot a spherical shell of thickness dk. So, we plot a spherical shell in k plane whose thickness is dk and we will see how many electronic states how many allowed states are there in this spherical shell.

So, the volume of spherical shell is as 4 π k^2 dk. So, the number of electronic states in these spherical shells will correspond to number of electronic states in energy range from E to dE and this is what we are trying to calculate actually. So, the volume of spherical shell is $4\pi k^2 dk$ and volume of single state is $\frac{\pi^3}{V}$.

So, the number of states in the spherical shell would be, number of states in the spherical shell would be the volume of the spherical shell divided by the volume of one state which is essentially $\frac{\pi^3}{V}$, pi cube by V. So, this becomes $\frac{4k^2 \mathrm{dk}}{\pi^2}$ V.

So, these are the number of electronic states in energy range dE number of electronic states in energy range from energy E to E + dE is $\frac{4k^2 \mathrm{dk}}{\pi^2}$ V. Number of electronic states per unit volume of the solid would be $\frac{4k^2\text{dk}}{\pi^2}$. Now, this right hand side is in terms of k we need to convert it in terms of E and for this we will use our E k relationship that we discussed on the previous slide ok.

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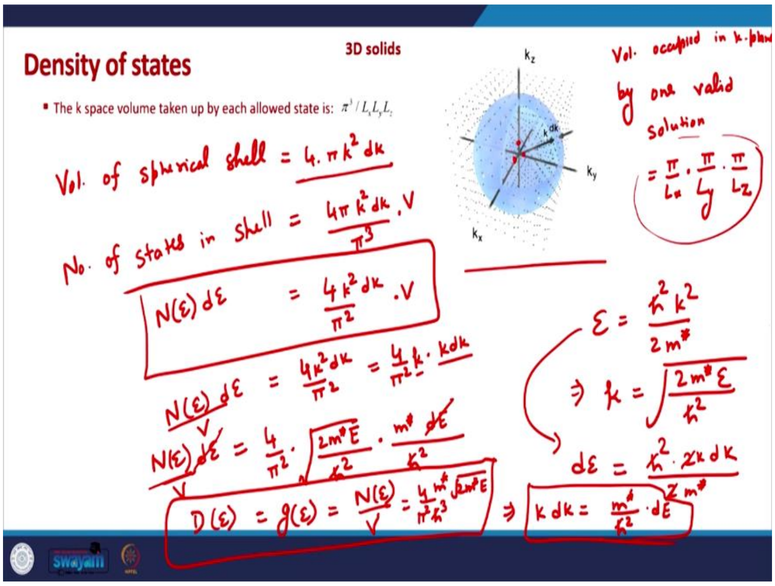

So, the E k relationship that we take is $\frac{\hbar^2k^2}{2m^*}$. So, which means k is $\sqrt{\frac{2m^*E}{\hbar^2}}$ this is k apart from this dE is now $\frac{\hbar^2 2kdk}{2m^*}$. If we differentiate this on both sides so, which means k dk is $\frac{m^*}{\hbar^2}dE$. So, in place of k^2dk we can sort of write k times kdk and this kdk value can be taken from here and this k value is this.

So, the number of electronic states from energy E to E + dE would be $\frac{4}{\pi^2}k.kdk$ that is $\frac{4}{\pi^2}\sqrt{\frac{2m^*E}{\hbar^2}}\frac{m^*dE}{\hbar^2}$ ok. So, dE and dE will cancel out. So, number of electronic states at energy E would now be given by N(E) and the density of state which we generally denote by D(E) or sometimes by g(E) will be number of electronic states per unit volume.

So, this is the number of electronic states per unit volume which is essentially this expression $\frac{4m^*}{\pi^2\hbar^3}\sqrt{2m^*E}$. So, this is how we calculate the density of states in a 3D channel we will discuss more about this in the next class. Please, I would request you to go through this derivation again and I will again quickly review this in the next class. This is an important derivation which will be useful at many places in our device analysis. So, see you in the next class.

Thank you.