Semiconductor Optoelectronics
Prof. M.R. Shenoy
Department of Physics
Indian Institute of Technology-Delhi

Lecture-5
The Density of States ρ(k), ρ(E)

We will continue with our discussion of the density of states.

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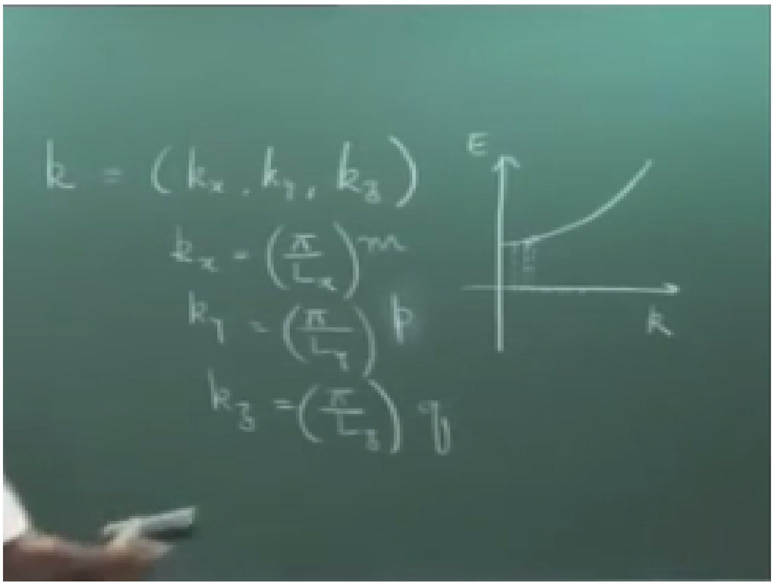

In the last lecture we have seen that k a state is characterized by k which has components kx, ky, and kz and by applying the stationary state boundary condition we have seen that kx, ky, kz are descriptized. So if you have a material of dimensional Lx*Ly*Lz, then kx is integral multiple of 5/Lx, ky=integral multiple of 5/Ly and kz can take values which are integral multiples of 5/Lz.

So fine to note is just a second made a mistake I had used p, so p and small p and q, where m, p, and q are integers. So the point to note is the values of kx, ky, kz are discretized and therefore k is discretized. By implication is that in the E-k diagram that we have the E-k the values of k which we have here are discrete values and corresponding to the discrete values we have discrete energy values.

Corresponding to each k value we have discrete energy value, however we have seen that the number of points here is very large, each of these value varies from a border of 1 million and therefore the number of points are very large essentially this forms a continuum. So that is why we normally draw E-k diagram continues E verses k.

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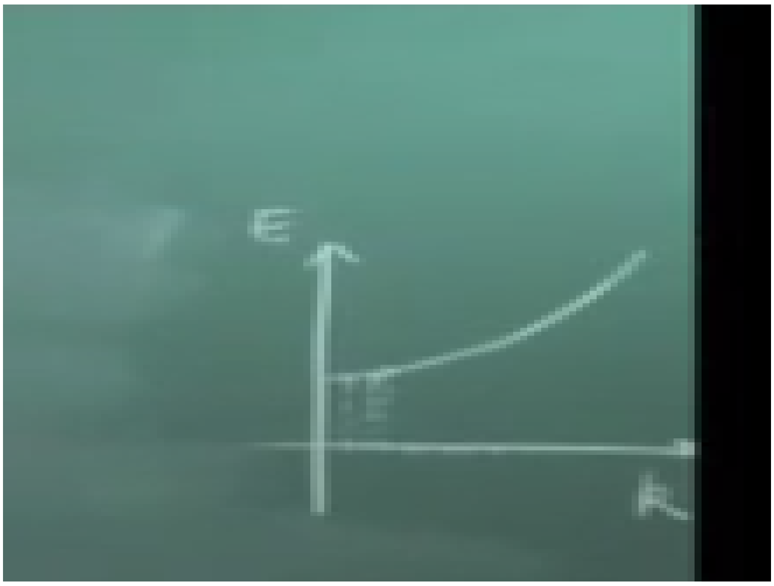

The second thing that we have seen is therefore in that k phase this is the E-k diagram, in the k phase or in the momentum space we have the number of permitted points, this is a k space which means the axis are kx, ky and kz. The number of points that we are enormously large number of points here and illiteracy every point here represents an allowed k value, every point represents an allowed k value.

Objective is to determine the density of states which means the number of points between k and k+dk per unit volume of the material. So how to determine that. So to determine is first thing we have applied stationary wave standing wave boundary conditions which means if I take a kx value if positive kx here the negative kx direction is automatically taken here, k in general represents the direction along which the electron is propagated is the propagation better.

Now if I consider the positive direction the negative direction is automatically taken care of because we had applied standing wave boundary condition, standing comprises of a wave which is moving in a forward direction and backward direction resulting in the standing wave. Therefore whenever I have taken a +kx, –kx has already been taken care, therefore we need to when we count the number of points that to get the density of states.

We need to take a positive values of kx, ky, kz only, it means in the k space which is a sphere we need to consider only the positive optent we see a square you have hemisphere, and then one fourth of that, that is the optent, only the positive potent which means you need to consider an optent which is like this.

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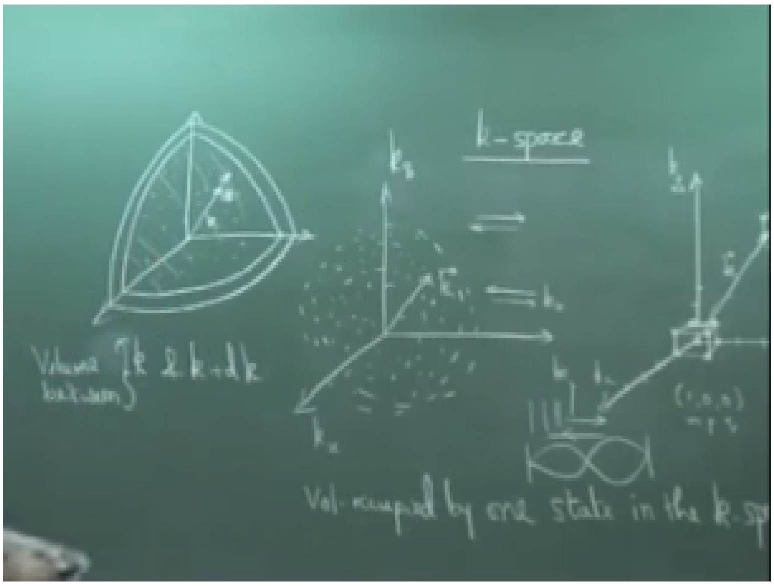

So this optent is generally represented like this, the sphere that is one eight positive part of the sphere. So this is that portion of the sphere where you have only kx positive ky, and kz that is this portion of the sphere, and also you can imagine is the potent one eight of the sphere. So you have half sphere, half hemisphere which you divide into 4 quadrants then you get one optent of this sphere.

The optent we have positive kx, positive ky and positive kz values. It is sufficient for us to consider only the positive k values k components. Because the negative k component is already taken into account when we go the standing wave boundary conditions. Now we have to count the number of points between k and k+ details, now before I proceed to count the number of points in the k space what is the volume occupied by one point or what is the volume occupied by one state.

I should not say one point one state, please see that if you draw a third diagram to make it more clear. Because I will show here a little bit spread out the point the permitted values, I want to draw the q, just for a second, so let macro environment we need height, so what I have drawn is each point here corresponds to a permitted value of k, you see what is this point, this point is 1, 0, 0, this point that is kx where m=this is m, p, q. So M=1, so this point is kx is phy/Lx and in this point ky and kz are 0.

If you take this point it is 0, 1, 0 and if you take this point this is 1, 1, 0 and this point here is 1, 1, 1. So different values of m, p, q will represent different points, you can take anywhere a q in general. So if I take k value here then there is a small spread to this side, there can be a small the next value. So let me show you first what I have drawn is a infinite civil volume in the k space.

In the k space a small volume this is a k value just see the picture if I change the ky this is ky, this is kx and this is kz. If I change ky/this separation which is phy/Ly then my k vector the tip of the k vector can sit here, the tip of vector can sit at any format here, the tip of the k vector because the k vector is defined by m, p, q values of marketing process, if you keep m constant k, p constant and change q then it will change by 1 unit in this direction.

So different values of m, o, q corresponding to different points in the k space, one point here is there by 8 different cubes, one point is shared by this is one cube for example this cube this point is shared by this cube with the cube on this side, let the cube on this side and 4 cubes below and other words every point is shared by 4 cubes assuming that Lx=Ly=Lz is a cube, what is the volume of this cube here.

The volume is phy/Lx*phy/Ly*phy/Lz phy/Lz or this is the volume of the cube, the volume I will make a statement and then you see the volume of one state one allowed state in the k space the volume occupied by 1 allowed state in the k space is given by this phy/Lx phy/Ly*phy/Lz. Y one state the state there are 8 possible states here because there are 8 corners, however every corner here, every point here is shared by 8 different cubes.

In other words it is just like when you consider the number of atoms in a cubic lattice you have one atom shared by 8 cube exactly like that k it is not atom these are simply points, what are these points, these points represent allowed k values, which means if you connect here to the origin to any of the point that will be an allowed k value, and therefore the volume occupied by 1k state.

In the k space this is we are all we are discussing in the k space in the k space is so the statement is volume occupied by 1 statement one state in the k space, in the k space=phy/Lx*phy/Ly*phy/Lz. In the k space if I find out what is the volume between k and k+dk, k and k+dk volume between k and k+dk I find the volume and divided by volume occupied by 1 states we give me number of states between k and k+dk.

Volume in the k space between k and k+dk/volume occupied by one state will give me the number of states between k and k+dk for unique volume will give me density of states. So the volume of between k and k+dk, please see this it means I am looking at a shell volume between this shells 2 shells, so one is this shell which is k this shell means this point is line on the first shell here k.

And the second one is between k and k+dk, this is dk, so the second one here that is this point is lying on the first shell and this is lying on the first shell, please imagine the 3D is so optent. So one of them is one of the k is sitting on 1 shell and k+dk is sitting on the next shell, what is the volume between these, what is the volume between that, how do we get the volume.

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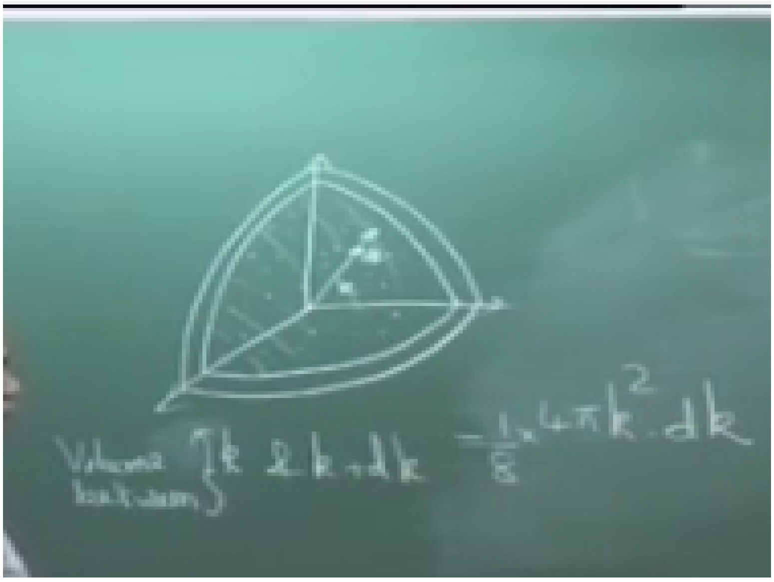

The volume between k and k+dk, so this is equal to 4phy a square, 4phy r square is a sphere, surface area of the sphere, multiplied by the thickness gives 2 volume of the shell, so 4 but we are considering only one optent of the sphere and therefore 1/8*4phy k square dk, volume between k and k+dk of the shell of the positive optent of the sphere is 1/8 of this.

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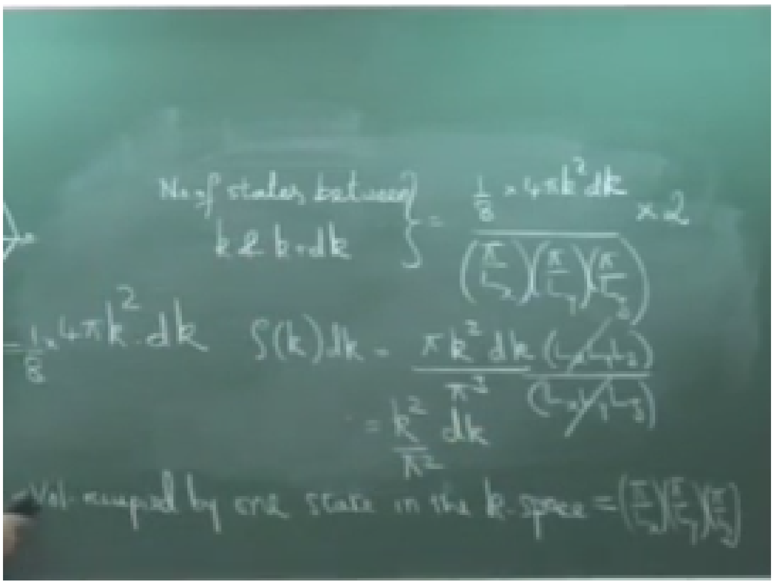

This volume divided by the volume occupied by 1 state will give me the number of, so the number of states between k and k+dk=1/8*4phy a k square dk/volume occupied by 1 state, that is phy/Lx*phy/Ly*phy/Lz. This gives me number of states, we have 2 add multiply this by a factor of 2 because we are considering momentum states of electron, electron can have 2 spin states which also contribute to the momentum states.

And therefore you have to multiply by this factor 2 because here state refers to momentum states of electron, it is a k space momentum space. So this is to account for spin of electron. So this is the number of states between k and k+dk, this give per unit volume is the density of state. So density of states, row of k, density of states, row of k, dk=this divided by Lx, Ly, Lz, that is the volume.

So you have 1/8*4*2, so that has already gone. So we have phyk square dk/in the denominator there is phy cube and in the numerator we have Lx, Ly, Lz here divided by volume which is also Lx, Ly, Lz, this is volume occupied by 1 state in the k space, this Lx, Ly, Lz is the physical volume, Lx, Ly, Lz is the volume of the material, a material of dimensional Lx, Ly, Lz volume that is the volume is this. This was volume in the k space.

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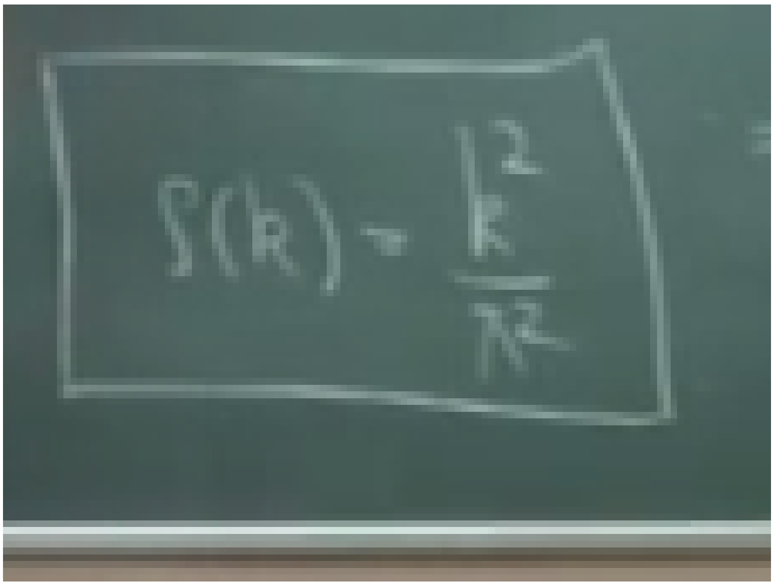

$$\boxed{\rho(k) = \frac{k^2}{\pi^2}}$$

So this gives me the density of states. So what you have what is left is simply this equal to k square/phy square*dk. I am sure many of you would have done this derivation earlier. Therefore we have the density of states, row of k=k square/phy square**.** So just if you know the definition correctly this is elementary algebra we have calculated volume and density by elementary. I have provided you have the definition clear and the basic picture clear, but there is nothing to remember here in this derivation.

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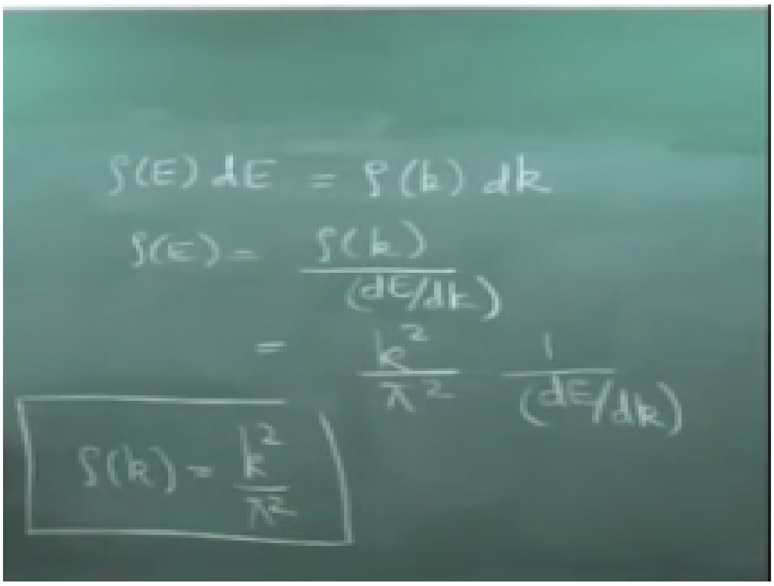

$$\rho(E)\, dE = \rho(k)\, dk$$

$$\rho(E) = \frac{\rho(k)}{(dE/dk)} = \frac{k^2}{\pi^2} \frac{1}{(dE/dk)}$$

$$\boxed{\rho(k) = \frac{k^2}{\pi^2}}$$

Just the definition has to be correct and simply follow the procedures is just 3, 4 steps. Now row of k is the density of states in the k space, but normally we need the density in the energy space because all the rest of the parameters which we get like the probability of occupation which is given by the Fermi function that is also in the energy state. So we would like to have the density of states in the energy state which means row of E.

How to get row of E, we know this k already seen row of E=row of k dk, the number of state between k and k+dk=number of state between E and E+de, that is what we have seen in the last class from the E-k diagram. Therefore row of E=row of k, I can write this as de/dt which is equal to k square/phy square*de/d one 1/de/dk. We make use of the parabolic approximation in very simple algebra.

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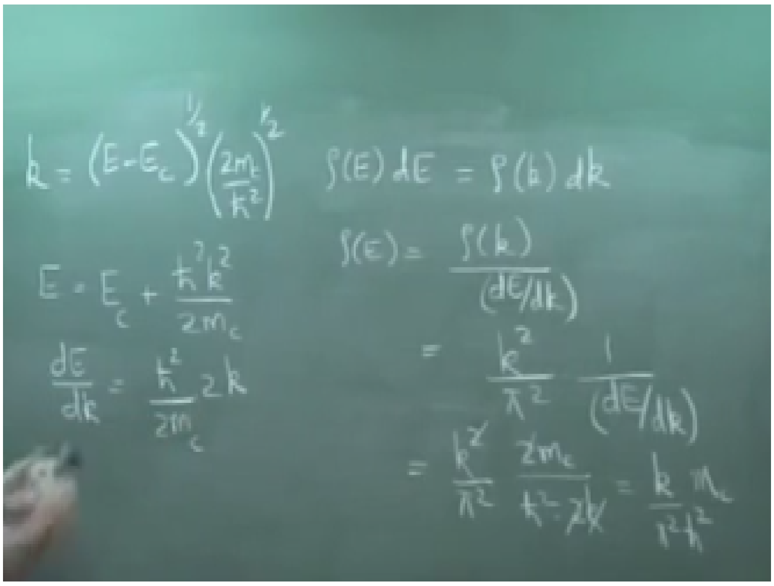

$$k = (E-E_c)^{1/2}\left(\frac{2m_c}{\hbar^2}\right)^{1/2}$$

$$E = E_c + \frac{\hbar^2 k^2}{2m_c}$$

$$\frac{dE}{dk} = \frac{\hbar^2}{2m_c}2k$$

$$\rho(E)\,dE = \rho(k)\,dk$$

$$\rho(E) = \frac{\rho(k)}{(dE/dk)}$$

$$= \frac{k^2}{\pi^2}\frac{1}{(dE/dk)}$$

$$= \frac{k^{\cancel{2}}}{\pi^2}\frac{2m_c}{\hbar^2 \cancel{2k}} = \frac{k\,m_c}{\pi^2\hbar^2}$$

As we saying we usually consider the electron and hole state where the parabolic approximations is a very good approximation. So we know the energy of electrons are given by Ec+h cross square k square/2 mc. Therefore E-Ec part let me to do de/dk here. So de/dk is this is 0, so we have h cross square/2mc 2mc*2k and what is k from this expression because I want to eliminate k completely.

From this expression k+E-Ec here E-Ec*2mc/h cross square, this is k square to the power of half 2mc/h cross square, this is k square, therefore k+this to the power half*this to the power of half. From the same expression just to rearranged k=this square. So I want to substitute for this k here, so we have this, so let we substitute hear therefore this is equal to first k square/phy square where by dE/dk.

So that is just this, so h cross square the denominator*2k*2k/twice mc, so 2 goes here, one k goes here, one k goes there. So we have mc/is a product, so I simply substituted this k square/phy square/2k*this. So this is equal to we have k/phy square h cross square*mc, I hope I do not make any mistake.

And substitute for k from here, so we have row of E=k, I will substitute this, so I have 1/phy square ok, I want to do something here, let me keep this 2 and 2 just because I want to take this together let we keep it as it is. So let me write this as 1/2phy square. There is 2mc/ h cross square, and let say 2 mc/h cross square to the power half, so this is 2mc/h cross square to the power 3/2*E-Ec to the power half.

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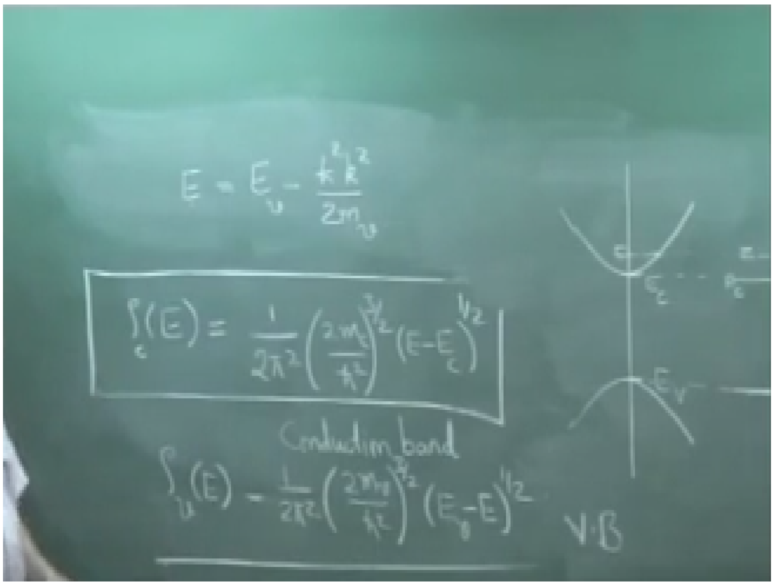

The expression for density of states in the conduction band. So normally this is designated as row c of E=1/2phy square*2mc/h cross to the power 3/2*E-Ec to the power half, what is this E here, is the energy of electrons in the conduction band which means if you look at the conduction band. So if you look at the conduction band where we have the E-k diagram you have the E-k diagram like this.

So this is Ec, this is Ed, we are looking at the density of states in the conduction band for E greater than Ec, E is any value here in the conduction band, any value here E in the conduction band, so E-Ec is this difference or if you compare this with your row band diagram then we are looking at the density of states available at an energy value E, so this is Ec the bang h and we are looking at an energy value E in the conduction band.

What is the density of state, so the density of state is given by this expression, it will be more useful to see what is the variation of density of states with energy E, but before that if you follow exactly what we have done is to obtain the density of states in the conduction band. If you follow exactly a similar procedure starting with for the valance band energy of holes in the valence band is EV-H cross square k square/twice mb.

Instead of using E=Ec+h cross square k square/2mc, if you use this and find out the density of states for the valence band you will get expression row v of E+1/2phy square*twice mv/h cross square to the power 3/2*Ev-E to the power half. Please derive this in the case simple exercise and you obtain the expression here. Now here we are talking of energy of electrons in the valance band here.

So E is less than Ev, that is why it is for Ev greater than E less than E, this quantities positive otherwise it will become imaginary, so E is less than Ev for the valance band. So this is for the valance band. These are the two expression for the density of states.

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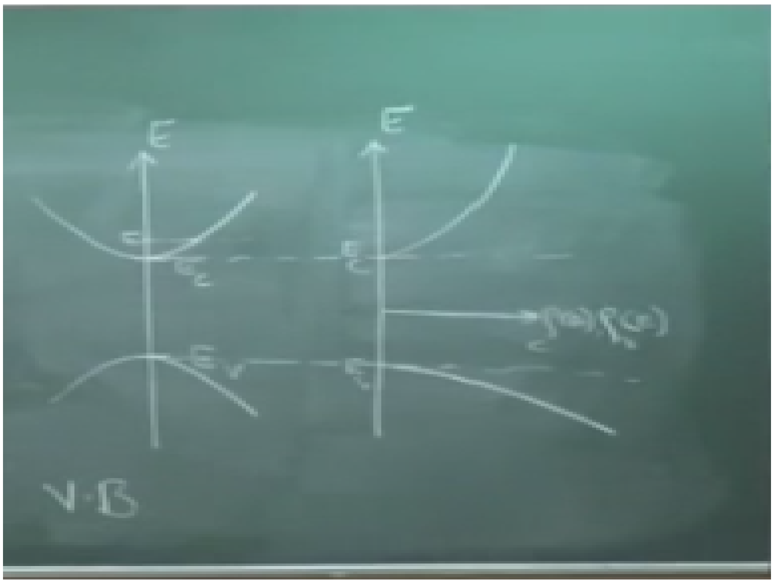

Now let me plot this how the density of states look like. So if this is E as I mention will always keep E on this axis, so we have all equivalent pictures E here and I want to plot row of density of states row of E and row of Environment So this is this value here is Ev, this value here is Ec, how does it vary with energy, all of these are constants for the conduction band only energy is the variable.

So it where is square root of E which means with E this would vary like this and similarly for the valance band this would vary like this. Please see again I have deliberately this is going rapidly like this here it is going the slopes are different because assuming that mv is different from mc, mb is much greater than mc, sometimes you see in the book the density of clock, density of states plotted like this.

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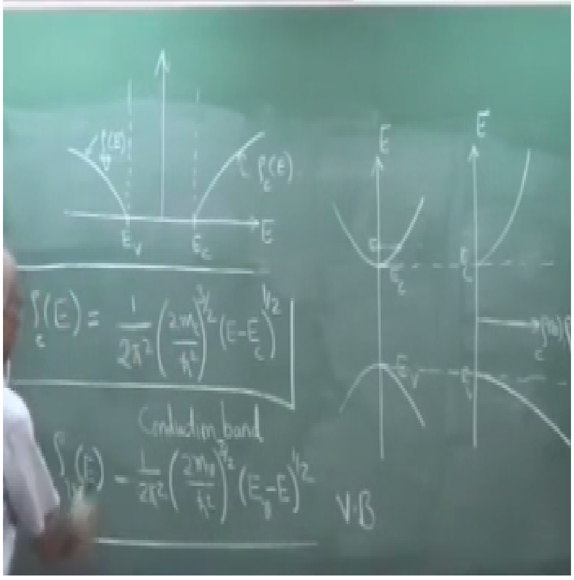

E here and you have Eb, and Ec like this, so it is square root of E variation, so this varies like this and this one varies, so this is row c of E, row V of E and this is row c of Environment So this is the density of states is now on this axis. But to keep a consistent picture we will plot always the vertical axis will remain the density of the energy. So this variation row c of E and this variation is row V of E.

The variation again depends on the effective mass the density of states available depends on the effective mass of the career is this alright. So these are expressions that we will need to calculate the carrier concentration because as I had already pointed out the density of states multiplied by the probability of occupation will give you the carrier density and integrated over the band will give you carrier concentration.

Before I proceed to we carry the carrier concentration and discuss about the probability of occupation I wish to draw your attention for to a small effect which is right here. The major discussions we will do a little later and that is related to the density of states in wuantum well structure.

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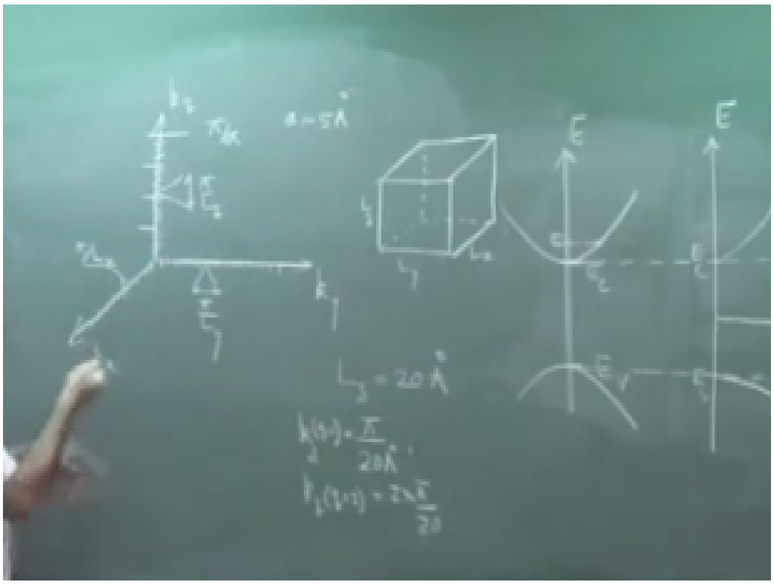

I considered a cuboid of dimensions Lx, Ly and Lz, this is Lz, this is Ly and this dimension of lx, the piece of semiconductor with dimensions this and correspondingly in the k space these are allowed values of ky, so this is kx ky and kz. They are very closely separated points, so starts from about 1 million points within the first zone very large number of points, the separation between 2 points here, so let me just zoom it and this is phy/Ly separation between two points here is this preparation is phy/Lz and separation between two points here is phy/Lx.

Suppose I reduce this dimension this was 1 mm let us say 1 mm I want to reduce this as I reduce this dimension that is we are reducing the vertical dimension here Lz, what will happen Lz is reducing which means the separation is increasing, I reduce it for the so the separation is increasing further and further. The maximum value of here was phy/k and k was approximately 5 and so on, that is why because Lz was 1 millimetre I had 1 million points here.

But if I reduce lz let us say Lz=20 Armstrong, I reduced 1 dimension to 20 Armstrong to thin sheet of semiconductor, what will happen, so the first point will be phy/20 Armstrong, this si kx kz the first pint kz which cube+1, so kz with cube=1 I have phy/Lz. The second point kz cuve=2 two times phy/20, so two times phy/20 Armstrong which is 2/10 Armstrong and cube=3 there is three times phy/20 and cube+4 is four times phy/20 which is phy/5 Armstrong which is nothing but phy/a.

The point is when have reduced this dimensions to 20 Armstrong I have only 4 permitted values 1, 2, 3, 4, the number of permitted values of kz are just 4, from 1 million it has come down to 4, you follow this but Lx and Ly is the same and therefore we have large number of points for Ly and Lx, but here it is completely discrete, with just 4 allowed states, what is the simplification.

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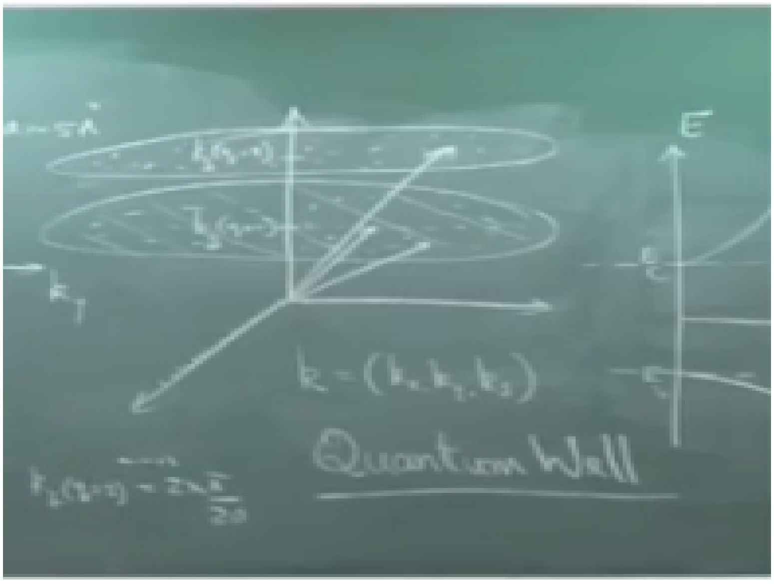

What will be the density of states, so I draw it again in the k space now I have first allowed point here, and second allowed point here. Let us say this is for kx or q=1 and kx sorry kz I am sorry kz q=2 where as these points can take as before very large number of points, very large numbers number of values permitted for kx and ky, but kz can for simplicity let us stay there are only two values it can be.

Because the thickness is very small, this thin sheet of a semiconductor how to be a quantum, we will discuss in detail a topic with slightly later, but at this point you assume that it is a quantum well but we will discuss about it. So this thin sheet corresponds to a quantum well as we will see, but the important point to see k values are highly descriptor what is its implication comprises of kx, ly, kz.

The first value of kz should be at this height earlier we had sphere because here large number of kz values also. Now the first value of kz should be at this height which means the k vector the tip of the k vector must lie on a plane receive this is axis imagine on a plane where kx take this value first value the k here, let me show this as a disk. So on this disk k can take any number of values any values.

But the tip of this must lie on this disk, see this disk is perpendicular to the kz axis, it has to lie on that because the first value of kz will be that, but the other values it can have any value of kx/k/k nay value but the tip must lie on this. We follow where will be the second value when will be the q=2 when it is Q=2 you will have a second disc, if you are not follow just hold on it will become clear.

All k values must have non 0 kx/kz, for propagating in unless you are propagating exactly in this scale then kz is 0, even if it is your propagating at any angle the first thing is a kz must have value equal to this which means it should lie on the first plane where else it can lie if k is sufficiently large that means the energy is sufficiently high remember that energy is a h cross square k square/2mc.

So if k is very large it means energy the kinetic energy is large, so electrons with large kinetic energy can have k here, the tip of the vector can sit either in the first plane or in the second plane more or less unlike in the previous case it was a sphere full of points anywhere you go. So that is why we have the volume of the sphere to find out the number of points. But now we cannot do that because k can sit either the tip of the k vector.

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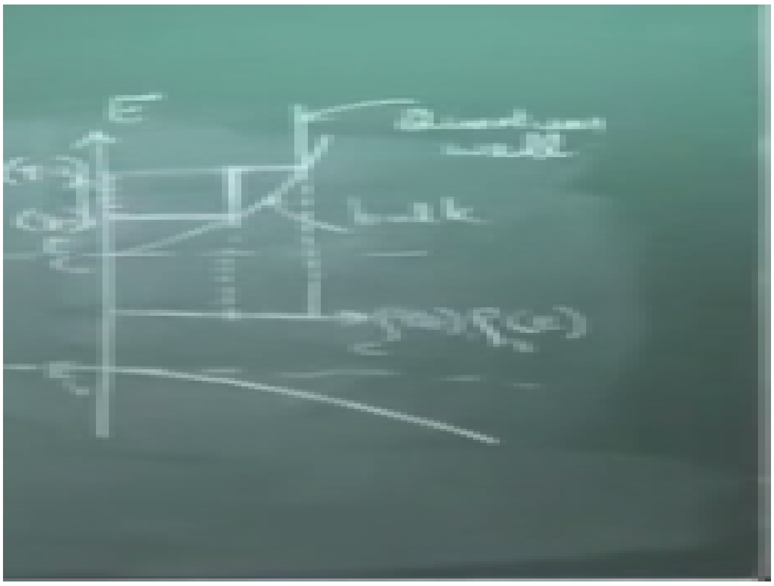

Remember k is a propagation vector can sit either in the first plane or in the second plane. How to calculate the density of states and what will be the density of states in a quantum well. So we will discuss this in the next class this is very important and the density of states let me see that the density of states will behave like step function. This is for the bulk, bulk semiconductor and the density of states for a quantum well.

So in the space the allowed states will remain on this part for different discrete corresponding to different discrete values of cube and they are well separated now or we q as also almost continuous and therefore the k would have been sitting anywhere. If you see in one dimension just if you see in 1 dimensions the k can or a value here which means the tip of the k vector can sit anywhere here like this it could or k can sit here.

The tip can sit here because there are no other intermediate value, so this is for q=2 and this is kz and this for q=1, k cannot take any value intermediate, the state are discrete and the consequence of this will be we will see that the density of state will remain constant up to some value of energy. So below was there is no state density of state this is the density on this axis remains it is constant here up to as you increase the energy here.

The density of state is remaining constant, it starts form here and please see the density of state here is constant in spite of the fact that you are increasing energy. When you reach energy value here this corresponds to q=1 and when you reach energy value corresponding to q=2 E corresponding to q=2 suddenly there will be a jump, why there is a jump because now the tip of the k vectors can sit on the second disc.

So earlier it could have been sitting only on the first disc, but now it can also sit on the second disc. If the magnitude of see if the length of the k vector is large then if you take the k vector like this it can easily sit on the second one, length of the k vector is large means the energy is large E-h cross square k square/2mc kinetic energy. So the larger the value of k it will get another disk to sit which means the permitted states become large.

Therefore at larger energy values the density of states is here in fact it is double earlier the density of here the density is double. But for all these energy the density of states remain constant and this has an implication in the device characteristics as we will see later that when we see semiconductor optical amplifier. So amplifier bandwidth will remain flat if the density of states remain flat, so we will see this discussion in the next class.