Semiconductor Optoelectronics
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Lecture-4
The Density of States

Good morning and we start with this lecture 4 the density of states, the topic is density of states.

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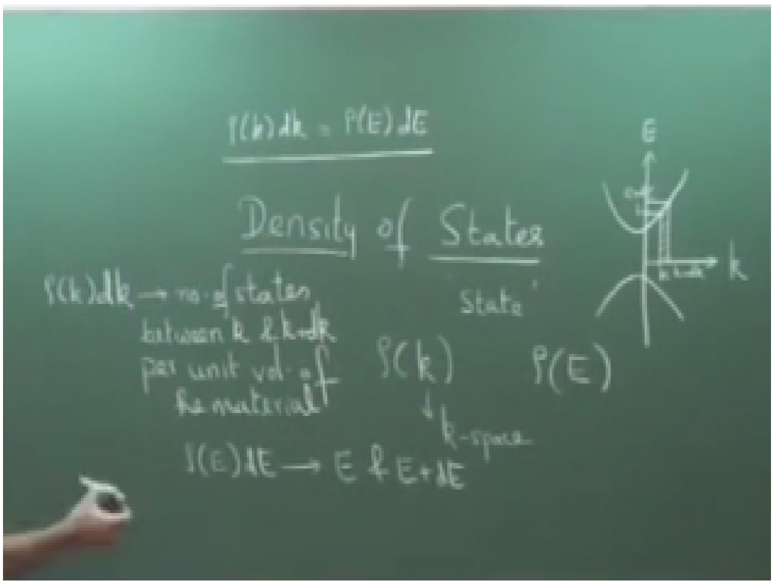

Usually the name indicates what it refers to density of state, for density this use as an idea that it must be something to do per unit 1 states what is the state, state is an allowed solution to the boundary value problem, states is a allowed solution which satisfies the boundary conditions, the general definition of state or a solution then Eigen solution or a mode different names are used.

But states is an allowed solution that satisfies the boundary conditions. So we are referring to the density of states in semiconductors which is row of k denoted by row of k or row of p. This is in case space row of k which is in the k space, what is this k and k space we will see row of k, row of e. Now row of k is defined as row of k dk, row of kdk is the number of stares between k and k+dk.

It is the number of states between k and k+dk per unit volume of the material. This is the definition of row of k, exactly like this you can also define row of e that is row of e de is the number of states between E and E per unit volume of the material, what are these E and k, E and k is the one which defines the band structure or the E-k diagram that we have seen in the last class.

So if you see a typical e-k diagram you can talk very well as you can see for every given value of k there is a corresponding to that I have a E value of key there is a k here and there is a E if I go to the next step that is k+dk then corresponding I have E-dP, this is k corresponding to that I have E value and if I say that this is k+dk then corresponding to that I have E+Environment

The number of states between k and k+Dk here, so what is this these are the allowed solutions allowed energy values as a function of k. So the number of states means the number of points that we get here in the E- diagram between k and k+Dk is the same as number of points between E and E+d. So obviously row of k dk=row of E use this shortly. This is the first picture of the density of states.

Before I proceed with the density of states and see what are the states, how many what is the number of states which is between k and k+Dk, let me call if you think from the E-k diagram that we have studied in the last class.

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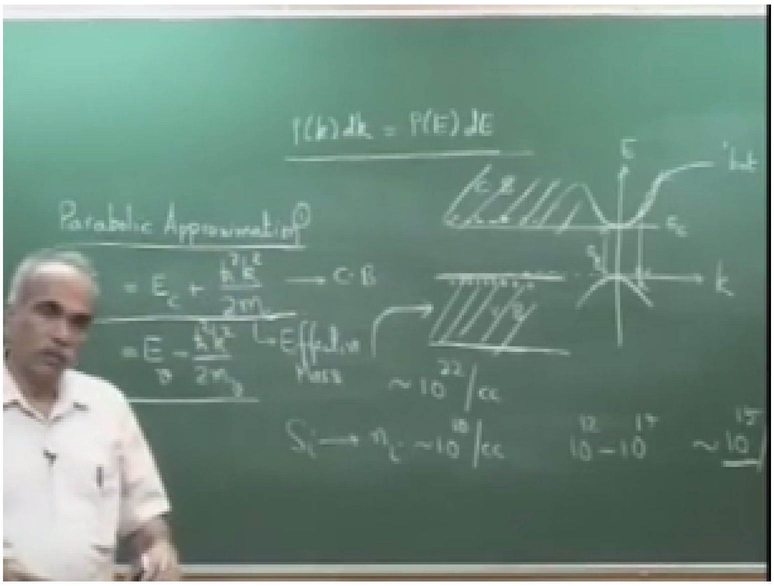

First point k E, this corresponds to as I shown of the this corresponds to the valence band and this corresponds to the conduction band, that is this is the energy value EC and here is energy value Ed and of course this is the band Eg. So this is the familiar band diagram, this is valence band and conduction band. We have seen that normally that the typical number of electrons in the valence band is of the same order as the number of atoms in the valence band which you have calculated in earlier lecture is of the order of 10 to the power of 22/cc.

The number of electrons in a band and generally if you take silicon for example intrinsic Silicon then the intrinsic carrier concentration ni at room temperature is of the order of 10 to the power of 10 to the power of 10/cc as I discussed in the last class it depends on the band gap and typical intrinsic concentration is this one, and if you drove a semiconductor to make a device say PN junction device.

Typical doping concentration could be anywhere from 10 to the power of 12 to 10 to the power of 17 which means the number of careers which are available is of this order or of the order of 10 to the power of 50. The number of careers which means the number of careers available in the conduction band here is the order of 10 to the power of 15/cc that devices which are heavily doped where it may be 10 to the power of 18 or 10 to the power of 10/cc is the carrier concentration.

In a band there are typically 10 to the power of 22 electrons and the carriers which are available which means the holes in a semiconductor valence band, hole in a valence band or electron in the conduction band is of the order which means it is much smaller compared to the total number of electrons in the band and therefore if we consider the E-k diagram, these careers which are available they are occupying only the bottom portion of the band.

We have holes here in the E-k diagram and electrons here which are literally in the bottom portion of the band because the number is so small they always tell to remain near the bottom which you have a hot electron this is the term used for electron hot electron, hot electron means electron with higher energy it will come down it will take till down by the phenomena call thermalisation.

We will discuss more about this later when we introduce first, so it will thermalize and come back to the bottom. Therefore in all devices when you want to analyse device characteristics normally it is sufficient if you know these the E-k variation near the bottom itself. Because almost all career the holes and the electrons are accumulated near the bottom and at the bottom here the variation is nearly parabolic.

This variation here is nearly parabolic and we use what is called parabolic approximation of the band parabolic approximation of the band which means the energy E the electron from the conduction band is given by E=EC+x cross square+k square/2mc square is where mc is the effective mass in the conduction band, effective mass of electron in the conduction band.

And Ev that is energy in the valence band, this is of the conduction band and for the valance bands this is given by Ev-H cross square a square/twice mV, where mV is the effective mass in the valance band in the effective mass of holes in the valence band. This is called parabolic approximation because as you can see the dependence of E is parabolic depends on k square it varies as k square.

That is why you can see this variation is like k square you see so anywhere if you go here for a given value a particular value of k here, then you have ec+this variations which is H cross square, k square by 2 mc. In the last class we discussed that by using the effective mass you can treat the career as a free particle. The kinetic energy of a free particle is given by t square/2n P square/2n. So the kinetic energy=P square/2m and P is H cross k, so we have H cross square, A square/2m.

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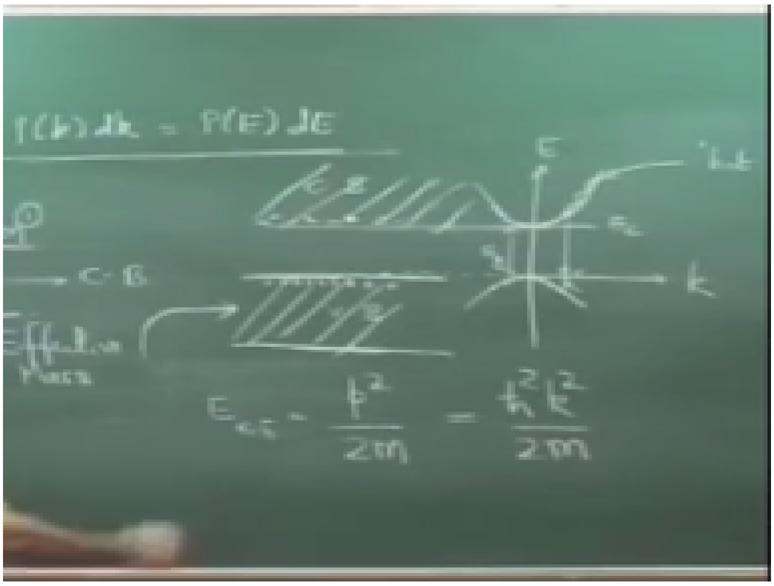

So here at the bottom of the band k=0 as about kinetic energy, but as you go to finite k value i have H cross square A square/2m and this is called parabolic approximation. if you see the hole band it will not go parabolic it will change it is the hole band, but normally if you are interested in the bottom of the conduction band and the top of the valence band this approximation is a very good approximation parabolic approximation ok.

First point and we will use this parabolic approximation in deriving the density of states because in most practical cases that is sufficient and as practicing engineer need do not worry so much about the figure but the second points that I discussed in the last class was the effective mass, which is also given by so N star that is MC or Mv depending on which was equal to 1/h cross square, b square/Dk square whole minus.

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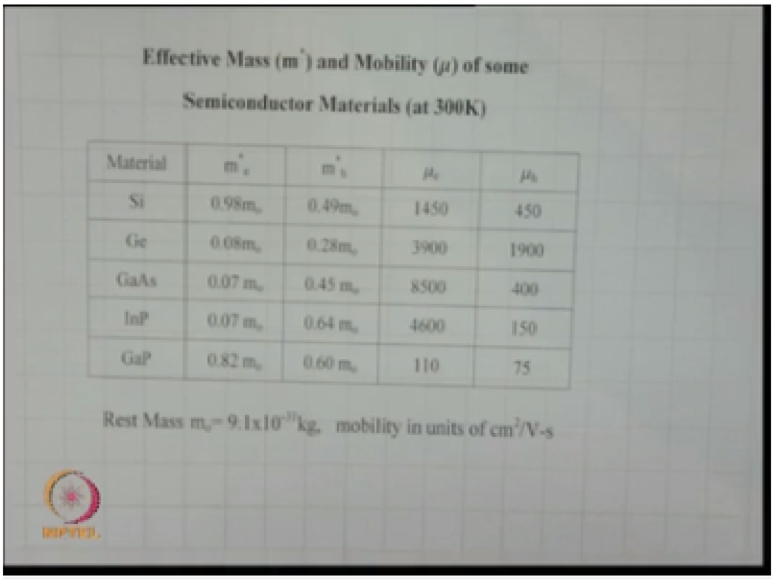

Effective Mass (m^*) and Mobility (μ) of some Semiconductor Materials (at 300K)

Material	m^*_e	m^*_h	μ_e	μ_h
Si	$0.98m_o$	$0.49m_o$	1450	450
Ge	$0.08m_o$	$0.28m_o$	3900	1900
GaAs	$0.07\ m_o$	$0.45\ m_o$	8500	400
InP	$0.07\ m_o$	$0.64\ m_o$	4600	150
GaP	$0.82\ m_o$	$0.60\ m_o$	110	75

Rest Mass $m_o = 9.1\times10^{-31}$kg, mobility in units of $cm^2/V\text{-}s$

Now I want to show you some typical values of ahh typical values of the effective mass in some semiconductor some of the semiconductor materials Silicon, Germanium, gallium arsenide, indium phosphide, gallium phosphide. These are widely used materials in optoelectronics, there are many more semiconductor suppose in optoelectronics these are some of the important semiconductors which are used.

What you notice is that the effective mass Silicon here in the conduction band and valence band the effective mass of holes in Germanium here is the value., in gallium arsenide you know that these are the value in fact there are something called light holes and high holes, but here we are mainly considering the high holes. I do not wish to introduce light holes and other bands at this stage.

So what I would like you to not give is also that smaller the effective mass larger is the mobility. We can see smaller the effective mass, larger is the mobility, mobility of electrons is much more compared to the mobility of force, so the band structure tells us an effective mass and it also tells us what is the corresponding mobility and what is the effective let us have a little bit more of this picture the rest of mass is M0 and effective mass is much small, it is like this effective mass is the mass experience or the mass exhibited by an electron. The mass exhibited by an electron when inside the semiconductor.

It is like you have a long wooden log, you try to drag it on the ground which is very hurry really hurry, we are not you not be able to drag it if the log is very big. Now you put that log in water and now you can pull it much easily because water buoyant force is giving an upward thrust and that log is feeling now much lighter and you can pull it without any difficulty.

It is acting as if it is a very light particle, it is why because it is in the medium that log is in water exactly like that then the electron is inside a semiconductor it is moving under the influence of the internal electric field. The electric field within the medium, so it has a pushing effect. So there are potential variations and electron is as if it is pushed and moving very smoothly.

That is why it feels very light and that is why the effective mass that you can see is much smaller in the conduction band, accordingly the mobility is much higher. Now let me come back to the density of states. So now we have to understand what is this k and what values can k get, we know that for every value of k there is a corresponding P value allowed energy value.

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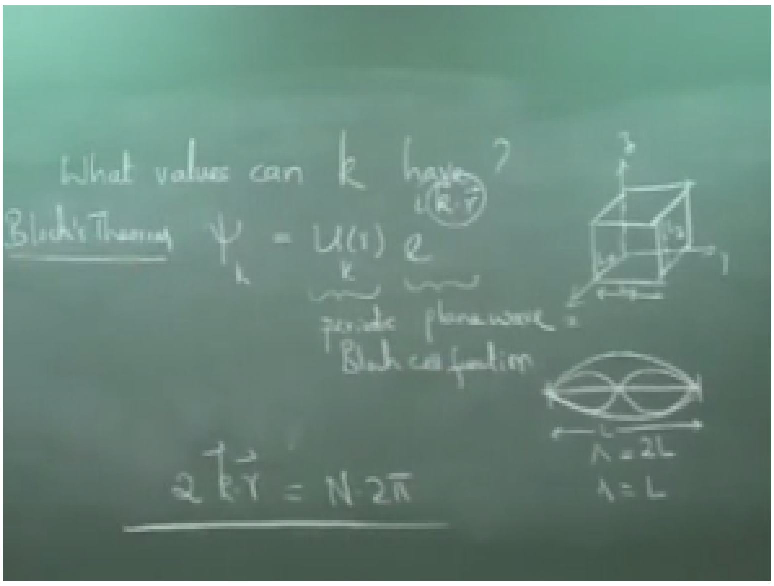

But what is the values that k can be, what are values in that k can be, what is this K and what values can K can be, the question is what values have what is this k and what value can k have. We call on log theorem that the wave function associated with electrons in a semiconductor phy k are given by Uk of r*e to the power of i k.r. K is a vector is a prorogation vector and not put the k notation here.

And this will bring more concepts about the k and the band structure itself because k is a propagation vector. So this is a plane way si a product of plane way and the block cell function which is a periodic block cell, block cell function, therefore phyk is periodic, now you know that the probability of finding an electron is equal to mod ph square. This is a periodic function.

If you consider a semiconductor a small piece of the semiconductor of dimensions so let me mark the axis. So this is x y z in space I have taken small piece of semiconductor let us say cubic or a cuboid. So this is of dimension lx, ly, and lz this height here is nz. So I am tellgin is qlx=ly=lz so let us say 1 mm size of semiconductor is small piece of semiconductor. The electron is bound to the semiconductor means you can find the electron inside but not outside.

Electrons bound to the semiconductor which means inside the same it is not outside, but we know that the probability of finding the electron is periodic it is oscillatory function therefore it is periodic. Therefore if the electron has to be found inside and not outside the probability is 0 outside which means size should go the 0 at the ends at the boundaries, which means the wave function should form standing wave in the middle. This is called a standing wave boundary conditions.

There are also periodic boundary conditions or stationary wave boundary condition. The logic is the field or the wave function has to go to 0 on the boundary of the which means if it has to go to 0 here and it has to go to 0 here and if it is period and oscillatory it means it must performing standing waves, it is like this you have a string which is strap towards that is base on 0 and it is given that it can oscillate periodically.

The displacement has to go to 0 which means it will oscillate either like this or like this which are the modes of oscillations of string between notes of oscillations of history what is the boundary condition that the displacement goes 0 at the two ends, that immediately restricts the oscillation period or the wavelength here as you can see this is the smallest wavelength here if I denoted by lamda=yl.

Because this is L, this length is l we see if I had a string of length L then this is half the wavelength and therefore lamda is equal to twice, in this case lamda=L, so lamda=L you can have many more such notes of oscillations of a string exactly like that in this case if the wave function has to form standing waves inside the 5 medium which means the face the round trip a please see that this is the face here r is the face e to the power of i phy.

Phy is the face, so k.r is the face and therefore twice k.r that is round trip face must be an integral multiples of 2. This is the condition for standing waves, round tip face must be an integral multiple of 2phy which means the way going from here to hear and coming back should add in face again before in 1 roundtrip the accumulated face should be integral multiple of 2phy.

So the condition is 2k.r=n times 2 k is a vector which means k=i times kx+jtimes ky+this is a unit vector ok let me put k times kz, k has 3 components, k director k=kx, ky, is the propagation vector, please see the space this is space if the electrons moving in which direction this is the k, it has controlled in this direction, in this direction and in this direction. So that x, y, z electron.

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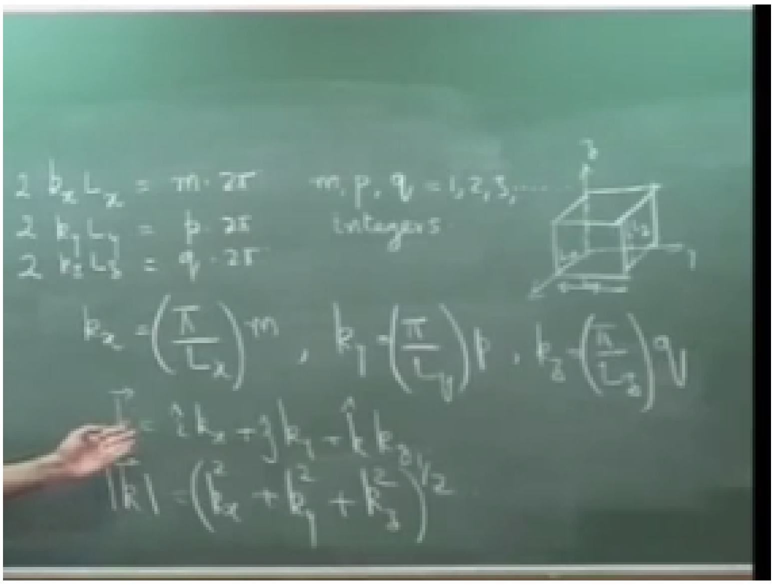

$$2k_xL_x = m\cdot 2\pi \qquad m, p, q = 1, 2, 3, \ldots$$
$$2k_yL_y = p\cdot 2\pi \qquad \text{integers}$$
$$2k_zL_z = q\cdot 2\pi$$

$$k_x = \left(\frac{\pi}{L_x}\right)m, \quad k_y = \left(\frac{\pi}{L_y}\right)p, \quad k_z = \left(\frac{\pi}{L_z}\right)q$$

$$\vec{k} = \hat{i}k_x + \hat{j}k_y + \hat{k}k_z$$
$$|k| = \left(k_x^2 + k_y^2 + k_z^2\right)^{1/2}$$

The electron could move like this it could move like this, so depending on that it will have different x, y, z components. If k.r=ntimes 2 phy which means that therefore because kx ky kZ are orthogonal components of k, orthogonal components of b, k.r=PC, what is k.k. k.r is kx+kyy+kzz, it is dot product k.r is kxx, ky/kzz. These 3 components here. Now if you consider this of dimensional lx, ly and lz then I must have twice kx*lx must be equal to n times integral multiple of 2ph twice kyly=3 times integral multiple of 2phy.

And twice kzlz=integral multiple 2 times, this for the vector and it has components x, y and z which are orthogonal components therefore if this is integral multiple of 2 by it means each of the components must also satisfy n terms 2phy p times to phy and p times to 2 phy and q times 2 phy and q times qphy where mpqr or them cannot be 0, so let me put 1,2,3 are you this means that kx=5/lx*m ky=phy/my*b and kz=phy/lz*qp.

And the propagation vector k=k cap or i cap kx+y cap j cap ky+k dash. So kkx a can take these values and per k is this and more k that is the magnitude of k=kx square +ky square+kz to the power r, more k+kx square, ky square, kz square. What is the point the important point to notice k comprises of three components and each of these components are now discretized, they are discrete which means the vector k itself is discrete.

We see kx ky kz take discrete values because m p and q are integers, if kx ky kz are discrete also be display what it means if we go to the k space now go to the k space now this si k space which means this is kx ky and kz, any vector k can be represented by these three components, but the k value itself k discrete values the separation between these is phy/lx because this is m=1 phy/lx 2phy/lx 3phy/lx and so on along y it is so this is phy/my this si twice phy/my and so on.

And similarly this is also distance, what is our objective is to determine row ok the density of states, the density of states is the number of states between k and k+dk per unit volume of the material. So we want to find out what are the values that the k will take, so in general the vectors k here will have an x component is here and y component it is this and z component this is. So this is the case when you are here or this vector k.

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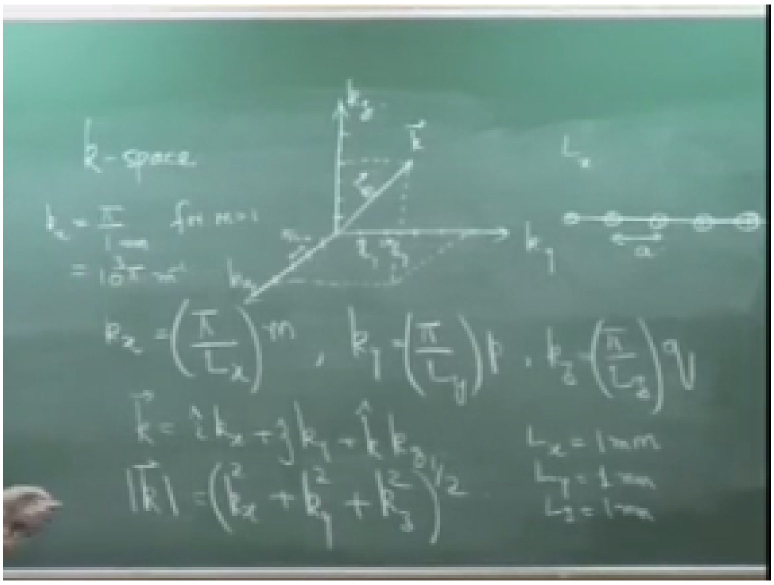

This is a vector k kx, ky and kz, to proceed further let us have an idea what kind of numbers will this be points will be there and what kind of numbers is this. If nx for example that the one dimensional k atoms are with interatomic spacing k, atoms are located periodically in a one dimensional lattice with an interatomic space k. What is lx if the dimension lx=1mm let us say we considered a cube with dimensions lx=ly=lz=1mm.

What is the smallest value of kx=1, so phy/lx, so smallest value of kx=phy/1mm, so 1mm for m=1 for m=1 which is equal to 10 to the power of 3 because 1mm 10 power -3metre 10 to the power of 3/meter inverse. This is the value of k, k has length inverse, dimensions of length inverse and as you can see this is the smallest value of k for a cube of side 1 mm kx, what is the largest value of k which is the largest value of k.

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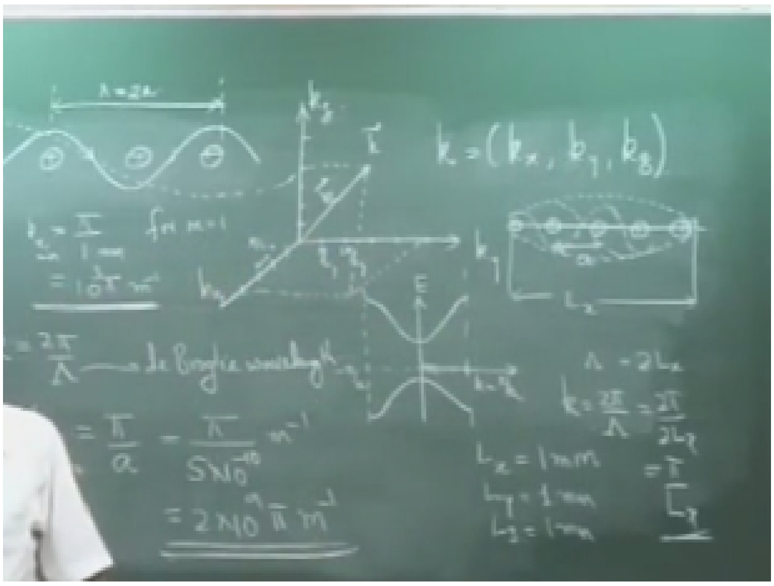

What do you think the largest value of k if you know that then we can know how many points will be there if like in the E-k diagram you recall in the E-k diagram that this is the boundary of the zone the first belongs if you consider the reduced zone picture then this value corresponds to k=phy/k and this si k=-phy/k and the reduced zone picture is the E-k diagram E verses k we have k=phy/k.

The largest value is k=phy/k, how do you get this k=phy/a, if you see this what is k=2phy/lamda, where lamda is the De Broglie wave, lambda is that a problem how do we imagine a lambda that electron which is the wave as this if this entire length is lx is the entire length then lambda the wavelength you can see wavelength lambda=twice lx or lx=half the wavelength, the dimensional lx=half the wave or lamda=twice lx.

Therefore k=2phy/lamda=2phy/2lx=phy/lx you see the same value I have got I am trying to give you a picture what could be specific stick picture why that is the smallest value k x is equal to phy/lx is the smallest value because that corresponds to an electron de Broglie wavelength which is like this from end to end, the fundamental mode in the case of a string. What is the largest value of to respond to smallest permitted value of lambda.

Smallest permitted value of lambda will be please see this is an electron the electron can go it can do like this or the electron wave can do like this what do you means by do like this which is if you assume electron which is entering from here to particle electron about the positive nucleus, so the electron bends towards the nucleus that gets scattered and it goes in this direction.

When the electron goes in this direction then the next positive nucleus which is attracting it so it starts bending towards this, it is getting attracted towards the positive nucleus here. So it can get attracted so much that it would again get scattered and start going in this direction but the next one will attract it and therefore the electron path, the path of the electron as a particle can adjust to this.

The smallest part, on the other hand if I have the electron coming from here it could slowly get scattered but if not bend so much, but it would slowly get attracted and it may bend like this and that corresponds to this that corresponds to a large wavelength, if it is attracted rapidly with the potential is strong then it could do this when it terms this what is the wavelength.

The wavelength here corresponds to from maxima to maxima distance and what is that this is interatomic spacing a and therefore this is equal to twice a, the wavelength lamda is equal to twice k, this is the wavelength of electron which is intertwined atomic spacing k therefore the smallest wavelength that you can have is this which means my k largest value of k=2phy/2a which is equal to phy value.

It is consist with discreet to that the edge of the first zone is k=phy/a, now why did I put this, the smallest value of k is this much, what is the value of k, so kx which means minimum value what is kx max=phy/a a-5 Armstrong which means phy/phy*10 to the power of 1-10 meter inverse which is equal to 2*10 to the power of 9/interring, kx varies from about 10 to the power of 3phy to the 10 to the power of 9phy, it varies by 6 orders of magnitude.

When you go from the minimum value here to the maximum value here, so form here 10 to the power 3 coming up to 10 to the power of 9, instead 10 to the power of 3phy in steps of 10 to the power of 3, what does that mean the number of points that you have here is a million 10 to the power of 3 to 10 to the power of 9, in steps of 10 to the power of 3, 1million points 1 million values of kx permitted.

And similarly Indian values of k y and million values of cases what is the point everyk is characterized by value of kx ky and kz each one can take a million value and therefore the combination can take millions of values. So the number of k values within 1 zone is the first band is do you understand this point and that is why I have put this number to tell you that number of points permitted number of k points permitted or of the order of million this one over this.

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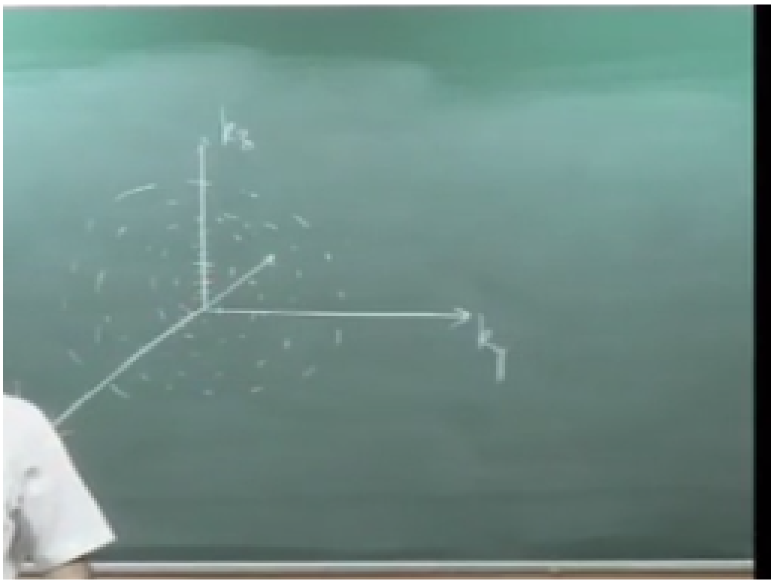

Because you are almost off you would have calculated this density of states and when you calculate you make an assumption that the number of points in the case we extremely large by putting these numbers the minimum and maximum I have illustrated that we need the number of k points permitted in the case space is extremely large. Therefore if you plot in the k space kx, ky, kz the million points here million points which means the permitted k value cab be there are enormous number of k values which are permitted in the k space.

What I am making every point here corresponds to a k value means the vector linking this to this point is an allowed value of k and such millions of point in the case you may continue from here in the next class.