# Micro and Nanoscale Energy Transport
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## Lecture – 12
## Fundamentals of Solid State Physics Part 1

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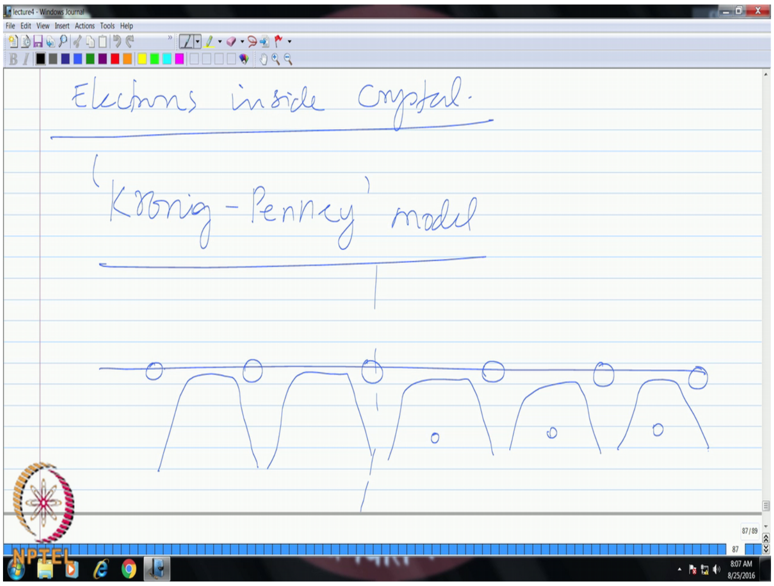

Electrons inside Crystal.

'Kronig - Penney' model

Good morning. Today we will look at a new topic that is we are moving away from the fundamental quantum mechanics of electrons in certain types of potential constraints to the actual behavior of electrons and real solids. So, as we discussed towards the end of the yesterday's class, one of the common way of describing the electron potential inside crystal is called the Kronig-Penney model. So, you can talk about you know the atoms distributed in the latish structure which forms the crystal in a one dimensional frame work and the interaction potential between the atoms can be represented like this and therefore, the electron moving within the crystal is actually constrained by these interaction potential. So, when we now look at therefore, real crystal which is periodic in nature we have to solve for the wave equation for the electron motion confined to this particular potential constraint.

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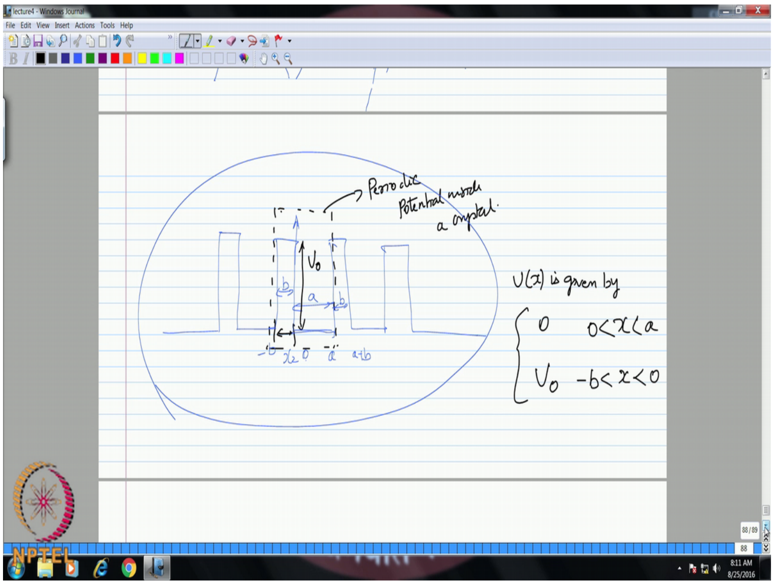

U(x) is given by

$$\begin{cases} 0 & 0<x<a \\ V_0 & -b<x<0 \end{cases}$$

In the Kronig-Penney model this interaction potential is further simplified by using the rectangular potentials of this particular form. So, essentially you can think about these quantum wells of width a and these are separated by means of small barriers of width b. So, this is basically the simpler representation of the actual interaction potential. So, this particular potential is therefore periodic, the periodicity is a plus b. So, every a plus b this potential keeps repeating. So, for our solution we will consider a coordinate system where we start the origin somewhere at the end of the potential barrier and we will have coordinate system where we take the potential barrier width. So, this starts from minus b to 0 is essentially the potential barrier width and from 0 to a is the quantum well width. So, this is one unit cell representation.

So, I will just mark the unit cell here. So, this is going to be the unit or unit cell or periodic potential inside crystal. So, we do not have to therefore look at all of these potentials together we can take one periodic unit cell potential and then we have to apply the periodicity boundary condition. So, the boundary condition here this, it is periodic at x equal to minus b and x equal to a, and apart from that you also have to give the boundary condition at x equal to 0. So, this is where the transition happens from the confined electron within the potential well to the free electron which can cross this barrier of width b.

Let us say that the height of quantum well, potential well basically is u naught. So, that is also the height of the barrier. So, the potential distribution u of x therefore, is given by; u of x is given by 0 for x greater than 0 less than a, that is inside the well right and you have potential barrier constraint u naught for x greater than minus b less than 0. So, now, we have to solve this Schrodinger equation with this for this particular periodic potential with this kind of constrains.

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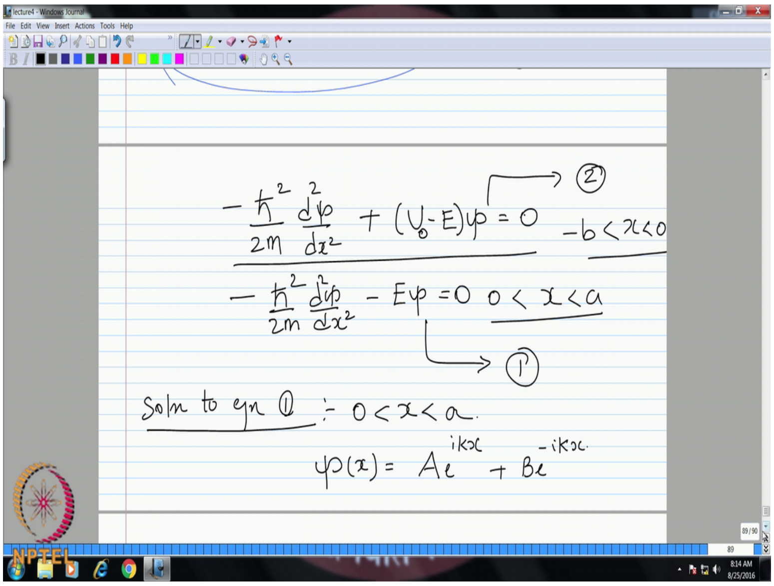

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + (U_0 - E)\psi = 0 \quad \xrightarrow{} ② \quad -b < x < 0$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - E\psi = 0 \quad 0 < x < a \quad \xrightarrow{} ①$$

Soln to eqn ① :- $0 < x < a$

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

So, can you again write down the special form of the Schrodinger equation? So, for this case again you have d square psi by d x square. So, then you also have the potential energy constraint in general case. So, we will be solving this for put u naught for the case where x is greater than minus b and less than 0 and then we will be solving the simpler form for the quantum well, is it clear.

So, therefore, what will be the solution for let us say this is 1, so the region 0 to a and the region minus b to 0 let us say equation 2. So, therefore, solution to equation 1 that is in the region 0 to a this is the quantum well solution. So, what do you get? We can write in terms of exponential functions. So, we have Ae power write running wave i K x very good, plus Be power minus i K x, good.

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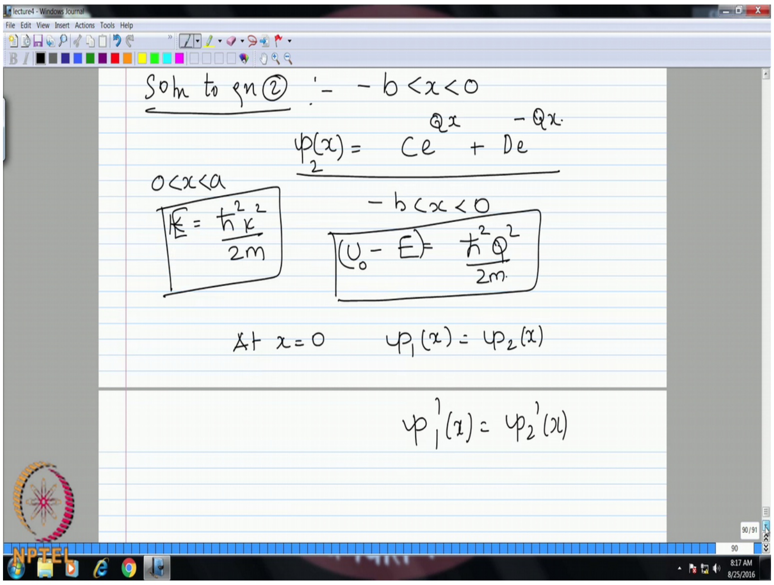

Soln to eqn ② :- $-b < x < 0$

$$\psi_2(x) = Ce^{Qx} + De^{-Qx}$$

$0<x<a$

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

$-b<x<0$

$$\boxed{(U_0 - E) = \frac{\hbar^2 Q^2}{2m}}$$

At $x=0$ $\psi_1(x) = \psi_2(x)$

$$\psi_1'(x) = \psi_2'(x)$$

And therefore, if you look at solution to equation 2 - this is the region beyond the potential barrier, potential constraint. So, the electrons with energy is greater than u naught can basically escape the potential constraint and they can move about freely. So, in this particular case what is the solution to equation number 2?

Student: (Refer Time: 08:22).

Yes because we have to put plus u naught minus e. So, therefore, we can write this as what?

Student: (Refer Time: 08:33).

C E power, we should use a different wave number now let us say Q plus De power minus Qx, so now how K and E are related to e. So, now, K will be or we can write E as h bar square K square by 2 m, this is in the region zero to a and now in the region minus b to 0 your U minus E will be h bar square Q square by 2 m u naught. So, this is the relation between your energy and your wave vectors K and Q, right. We have already seen this yesterday when we looked at finite potential wells.

So, now, again you have four constants and you need what four conditions to solve now we can apply the continuity of wave function and its derivative what x equal to 0. So, x equal to 0 is the point where you have transition between solution 1 and solution 2. So, you can this psi 1 psi 2 in fact, if you want. So, therefore, at x equal to 0 you can apply psi 1 of x should be equal to psi 2 of x and so are their derivatives, psi 1 prime should be equal to psi 2 prime.

So, this gives two equations for finding out two unknowns, but we have two more unknowns to be determined and we need therefore, two more conditions and what we can do. So, now, we go to this periodicity since this unit cell is periodic. So, we try to somehow; we know the potential is periodic, but how do we link the solution for a periodic potential. So, we use what is called as Bloch theorem, Bloch theorem.

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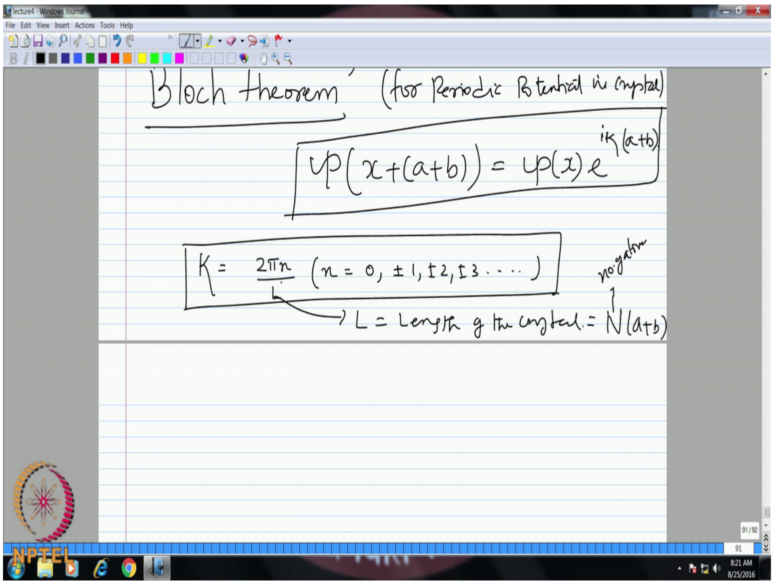

Bloch theorem (for Periodic Potential in crystal)

$$\boxed{\psi(x+(a+b)) = \psi(x)\, e^{i\kappa(a+b)}}$$

$$\boxed{K = \frac{2\pi n}{\phantom{L}} \quad (n = 0, \pm 1, \pm 2, \pm 3 \ldots\ldots)}$$

→ L = Length of the crystal = N(a+b)

no. of atoms

So, this gives you the form of the wave function that should be applied if your potential is periodic. So, this says that psi of x plus a plus b; that means, if you are looking at the wave function at some position which is periodic with a plus b the potential is periodic every a plus b, so after a plus b at that particular position this is linked to the wave function at x, as this into E power; now I am going to use kappa here; this is another wave vector not to be confused to with K and q. So, will come to that power multiplied by a plus b. So, this is your Bloch's theorem without going into the detail of its derivation so this for periodic potentials in a crystal.

So, the periodicity in the wave function is expressed in this particular format and what is kappa here? So, kappa is another kind of wave number this for crystal however, so what we have written as K and Q these are the wave numbers corresponding to the electrons. So, now, this kappa is the wave number corresponding to the crystal and this puts a condition again that it is not continues, but it is discreet given like this and n can be 0, plus or minus 1, plus or minus 2, 3 and so on. So, this is basically the kappa and what is L? L is the length of the crystal. So, it can be expressed as capital N into a plus b; that means, where n is the number of atoms. So, if you are looking at this potential that we have written here. So, it is periodic every a plus b. So, we have n number of atoms the entire crystal length will be n times a plus b. So, that is the length of the one dimensional crystal.

So, within this crystal this wave vector of the crystal will exhibit some kind of relationship. So, it is 2 pi n by l or n can be 0 plus or minus 1 plus or minus 2 etcetera.

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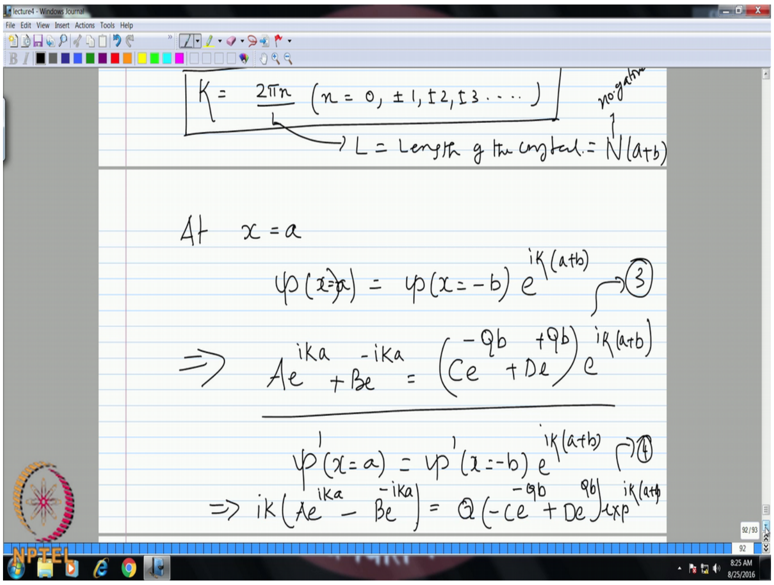

$$\boxed{K = \frac{2\pi n}{L} \quad (n = 0, \pm 1, \pm 2, \pm 3 \dots)}$$

$\to L = \text{Length g the crystal} = N(a+b)$ ← no. g atoms

At $x = a$

$$\psi(x=a) = \psi(x=-b)\, e^{iK(a+b)} \quad ③$$

$$\Rightarrow Ae^{iKa} + Be^{-iKa} = \left(Ce^{-Qb} + De^{+Qb}\right) e^{iK(a+b)}$$

$$\psi'(x=a) = \psi'(x=-b)\, e^{iK(a+b)} \quad ④$$

$$\Rightarrow iK\left(Ae^{iKa} - Be^{-iKa}\right) = Q\left(-Ce^{-Qb} + De^{Qb}\right) \exp^{iK(a+b)}$$

So, if you therefore, apply this Bloch theorem at x equal to a; that means, we are going to write the wave function at x equal to in terms of x equal to minus b, because it is periodic about a plus b. So, at x equal to a we are go in to apply Bloch's theorem which says that psi of x should be x equal to a should be equal to psi of x equal to minus b times exponential I kappa a plus b right. So, therefore, if you substitutes our wave functions will be getting Ae power ika plus Be power minus ika is equal to Ce power minus Qb plus De power plus Qb times E power i kappa a plus b. So, you have equation number 3. So, we had equation one these are the conditions, boundary conditions two, now you have periodic condition three and what should be the fourth condition. Again the derivatives also should fallow the same theorem. So, again you can apply this for psi prime at x equal to a should be equal to psi prime, x equal to minus b times E power I kappa a plus b. So, this should give you, can you all find this out, write it down? So, what do you have?

Student: ika (Refer Time: 18:13).

ika minus Be power minus.

Student: ika.

Is equal to Q into minus C E power minus Qb plus De power Qb times exponential I kappa a plus b. So, this is your condition number 4. So, therefore, I am not now going into further details you can apply these four conditions and therefore, find out the constants and I only write down final equation what comes out.

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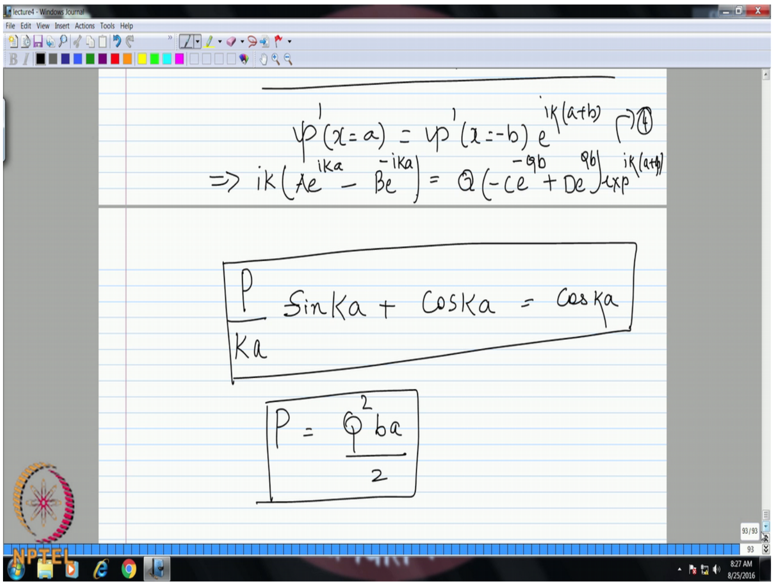

$$\psi'(x=a) = \psi'(x=-b)\, e^{ik(a+b)} \quad ④$$

$$\Rightarrow ik\left(Ae^{ika} - Be^{-ika}\right) = Q\left(-Ce^{-Qb} + De^{Qb}\right) \exp^{ik(a+b)}$$

$$\boxed{\frac{P}{Ka}\sin Ka + \cos Ka = \cos ka}$$

$$\boxed{P = \frac{Q^2 ba}{2}}$$

So, we can express P by Ka into sin Ka plus cos Ka is equal to cos kappa a, this is your final equation that you get to solve for Q 1 K. Now where P is nothing but Q square into b times a by 2, I am just clubbing this wave vector Q square times b times a. So, b is basically the width of that barrier, a is the width of the well divided by 2. So, this p is what is written here. So, you have a final equation which you can solve for getting the wave vector K.

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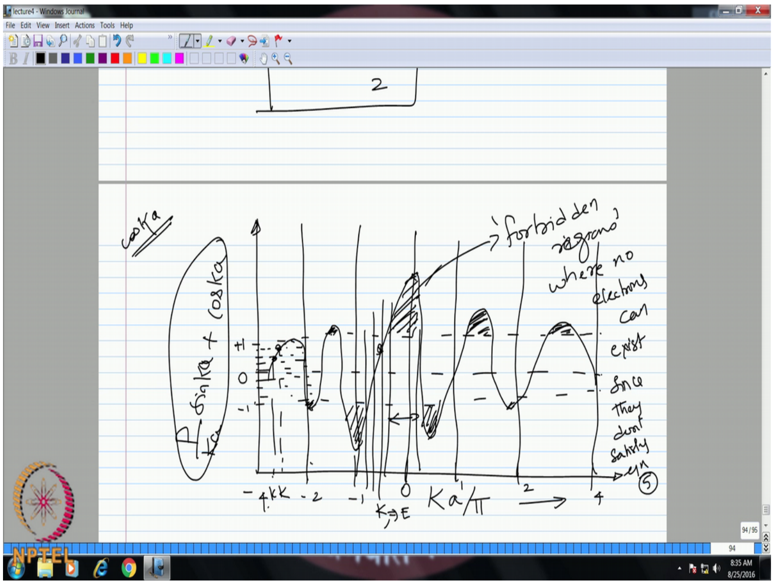

'forbidden regions' where no electrons can exist since they don't satisfy eqn ⑤

So, now if you plot this, how do we find the solution by plotting we can get the roots of this equation. So, we can actually plot on the x axis capital Ka by pi. So, this is some kind of non dimensional wave number, I am non-dimensionalizing the wave number as Ka by pi on the x axis and I am plotting this entire function on the y axis. So, to find out the roots of this equation, therefore, on the y axis I have P by Ka sin Ka plus I have cos Ka. So, if you plot this function, so Ka by pi can actually take also negative values. So, you have 0 1 2 4 and on this side you have minus 1, minus 2 and minus 4.

So, you can draw. So, this will be looking like. So, about zero it is symmetric and you have a P cut zero and then it goes about like this. So, this is how this function will look. Now if on the right hand side what do we have? Cos kappa a. So, what should be the maximum value minimum and maximum for this function? Plus 1 and minus 1, therefore, if you plot plus 1 and minus 1, this will be somewhere roughly you know 0 and will have plus 1 you have minus 1.

So, therefore, what is the region now in which you can find the routes? Only where they coincide, where values of cos kappa a will be equal to these values. Now there are values which are above plus 1 and minus 1 for this particular function that is if you shade it these are regions like this, now the regions are not possible because they are exceeding right hand side values. So, these are therefore called forbidden regions. So, you cannot have physical values of this function because they do not lie within this right hand side cos kappa a therefore they are not included in the final solution. So, this is the region where no electrons can exist because they are not satisfying let us say this is equation number 5 since they do not satisfy.

So, now what we can do is if therefore, you want to calculate the energy of the electrons, what do we do? So, we have to simply put vertical lines and then that would be giving the corresponding value of K which interned determines what is the energy. So, that energy is calculated using these relations right. So, all you need do is only look at the corresponding routes of K, the wave vector or wave number K and that will give you the energy of the electron. So, therefore, if you draw vertical line like this, you can therefore, find out the corresponding value of K for this and which can be translated into energy, similarly all these different lines.

Now when it comes to this forbidden region, there no electrons can exist therefore, you cannot have any values of energy there. So, now, what happened? From here to here you will produce a band gap, you understand. So, this is how when semi conductors, metals, we talk about the concept of band gap between two bands - valance bands, conduction bands, so how this band gap comes is because of this forbidden region.

So, when we now convert this and you should also understand that what I have drawn here are not perfectly continuous, cannot be continuous lines as well because the values of cos kappa a these are discreet because of the fact that K is kappa is discreet, right, kappa is discreet because it is 2 pi n by L. So, therefore, if you look at this here you will have discreetness, you will have this; you will have this like this. So, these are discreet solutions and wherever this point intersects here will be one value of K, you understand and where these cuts here will be another value of K. So, these are actually again discreet solutions. So, what we talk about solutions of K are themselves discreet values not continuous there, you can say cos a continuous and top of that you have this forbidden region which is quite discontinuous. So, this will result in the band gap or separation between the energy bands.

So, therefore, we can now convert this plot into a plot of energy verses kappa that is call the dispersion curve. So, people sometime use kappa and some text book it is just written as small K to distinguish it from K and capital K and q, capital K and q are the wave vectors for the electrons the kappa or small K is use to determine, is used to denote the wave vector for the crystal which is 2 pi n by L right. So, we can actually convert now this plot into a diagram for the energy bands, where I plot the energy E by E naught non-dimensionalizing the energy. So, where E naught is nothing but h bar square by 8 m a square this is some non-dimensional number.

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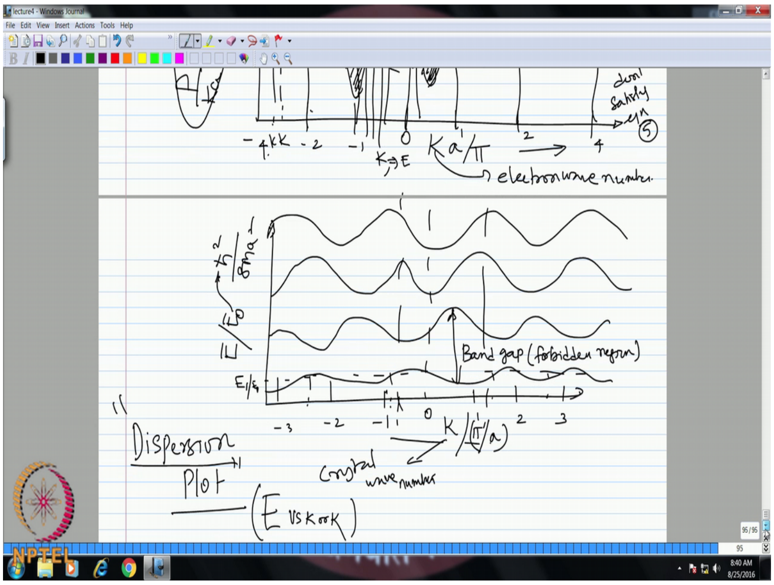

Similarly, I can now non-dimensionalize the crystal wave vector which will be kappa by pi by a, kappa a by pi - like the way I plotted here Ka by pi this is for the electron, electron energy. Now this is for the crystal. So, this is your crystal wave number. So, just to make sure you get confused this is your electron wave number and then what do you find is for a given value of energy you can have multiple values of these wave vectors. So, therefore, you can draw something like and once again you can mark the origin for this 0 and then you can have similar to this 1 2 3 4 and so on. Similarly you can have minus 1, minus 2, minus 3 and so on; that means, for a given value of energy you can say this value of energy E 1 by E naught you have multiple values of the crystal wave number. So, how do you understand that or how do you understand that. So, that crystal wave number values are basically these discreet lines. So, you draw vertical, so that is one given energy value of energy. So, one given value of energy can take multiple values of this kappa a, now we are converting that plot into an energy verses crystal wave vector plot. So, this plot is call the dispersion plot very important for solids.

So, finally, what it means is we are not interested in not only the individual energy diagram of the electrons, but for the entire crystal how this energy is dispersed. So, this is called the dispersion plot or capital E versus, people use either small K or kappa this is the crystal wave number. So, now, if you plot the next energy level for example, now, you will have this energy gap band gap coming into picture. So, wherever have this band gap you will have a big space. So, therefore, you can plot the next set of, this is basically your band gap coming from forbidden region. So, you miss all the values in the forbidden region you do not plot them and this creates the band gap and similarly you can continue this, this is all periodic so on and so forth.

So, now once again you see that these are all periodic because we are talking about crystal (Refer Time: 33:30) we are applied periodic potential, we applied periodicity of wave function to Bloch theorem. So, therefore, the solution is periodic values of the dispersion plot are also periodic. So, we only take one unit cell again. So, that unit cell is now extending for Ka by or kappa a by pi between minus 1 to plus 1. So, that is the unit cell about which the dispersion curve is also periodic and if you just plot only for that region.

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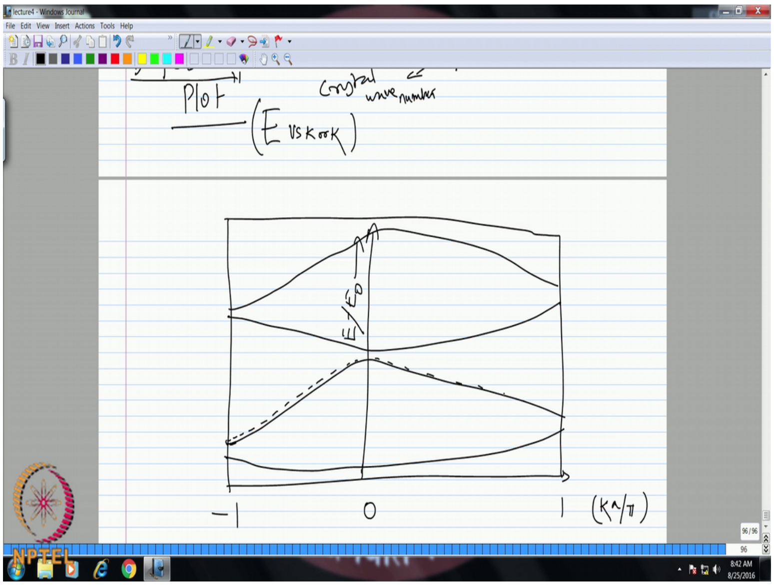

So, we are talking about minus 1, 0, 1, so we have kappa a by pi and we are plotting E by E naught. So, I will just a box, the lowest value will be something like this symmetric about zero and then you will have something like this, then you have a band gap and then you will have something like this and again you have a band gap, then something like this these are the different energy levels.

Now, also these are actually not perfectly continuous as I said you have little bit of discontinuity, if you really want to plot them it will be like this because your kappa a is also a discreet value, really speaking these are cos i continuous, but nevertheless you can assume them to be some solid line like this. So, you understand. So, this is how for a real structure the electron energy levels look. We started from calculating the electron energy levels in quantum well, now we have gone to a real structure and we have seen how the dispersion of energy level takes place in a crystal by applying so many conditions and finally, also this discreetness results in a forbidden region which causes these band gaps to appear.

So, now how does this influence the filling of electrons and how this can be use to classify material? So, this is what we will quickly do now in the 10 minutes. So, now, if you see look at the periodicity of this dispersion curve between minus 1 to 1, it is symmetric about zero therefore, even if you depict for one half maybe from 0 to 1. So, that should be simply a mirror of the other side. So, therefore, to in order to classify materials I will just give an example of how these energy levels are filled for different materials and that is how they are actually classified.

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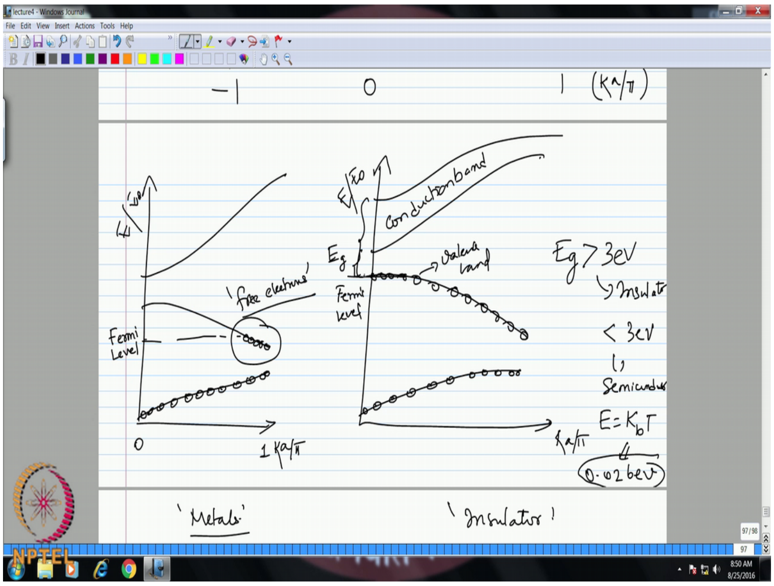

So, if you for example, first, I am only drawing the positive quadrant. So, you have kappa a by pi from 0 to 1 and you have E by E naught on the vertical axis. So, this will be looking like this, this will be looking like this and this will be looking like this. So, I have just drawn 1 2 3 for 0 to 1.

So, first if you take the case of metals, if you take the case of metals what do you find? The electrons are filing all the lower energy levels from the lower energy levels it keeps going, now you have a band gap, but the electrons do not have a problem in metals. So, at 0 Kelvin if you look at till what level they are filled? So, this is called the Fermi level. So, Fermi level tells you what is the maximum energy to which the electrons are filing the energy level at 0 Kelvin. So, you will see that in metals already some electrons have occupied the second energy level, energy state and the rests all vacant; that means, now if you keep increasing the temperature these electrons can freely move within this particular bend without any problem and therefore, all these are what? Conduction electrons or free electrons, in that case this becomes the conduction band.

So, you have to therefore, look at the Fermi level and from then onwards you will decide what is the valance band, what is the conduction band. In this case conduction band you have plenty of space to move the free electrons. So, therefore, these are behaving like metals, they are very good conductors of heat and current.

So, if you then go to the case of an insulator. So, I am you can draw another one - E by E naught kappa a by pi. So, now, you are going to describe how these states are filled. So, in the case of insulator what do you think will probably happen? It is not that it should be only filled till here it can also occupy this energy level at zero Kelvin. So, then this could be the Fermi level at 0 Kelvin, now this will be the position for the case of insulator, now what happens? You have band gap E subscript g band gap in the energy separation. So, at zero Kelvin this is your condition. So, therefore, at higher temperature, but the problem is this band gap is too much in insulators, in semiconductors this can jump. So, therefore, then this become your conduction band and this is Fermi level, end of Fermi level now will become this band will be the valance band; that means, valance band is completely filled and conduction band is totally empty divide of any electron. So, therefore, there are no free electrons.

So, this band gap is too much, now we are saying that band gap looks may be looking small, but I have probably drawn this for a semiconductor here, but if you are looking at real insulator the actual conduction band can start from where here. So, then this could become your band gap. Therefore, a typical thumb rule if your band gap is greater than three electron volts between the valance and conduction band, this result will result in material becoming an insulator. If it is less than three electron volts, this will be a semiconductor. In fact, the energy at room temperature K b T if you calculate in electron volt this will be 0.026 electron volts so; that means, if this has to be a semiconductor at room temperature the band gap should be of this order for the electron to overcome this band gap, otherwise it will be semiconductor at a higher temperature. So, we talk about room temperature semiconductor; that means, there band gaps are of the order this size, of this electron volts.

So, again in semiconductors you have different classifications you have intrinsic type and you have extrinsic type and all these are now going into electrical engineering, but I am still because you should at least understand how they look, now beyond that we are not interested. So, in the case of intrinsic is what we are talking about a band gap which is comparable to the K b T whatever temperature you are talking about. So, then they can naturally transition by themselves, but they need an external help. So, they become extrinsic semiconductor, and how that will work?

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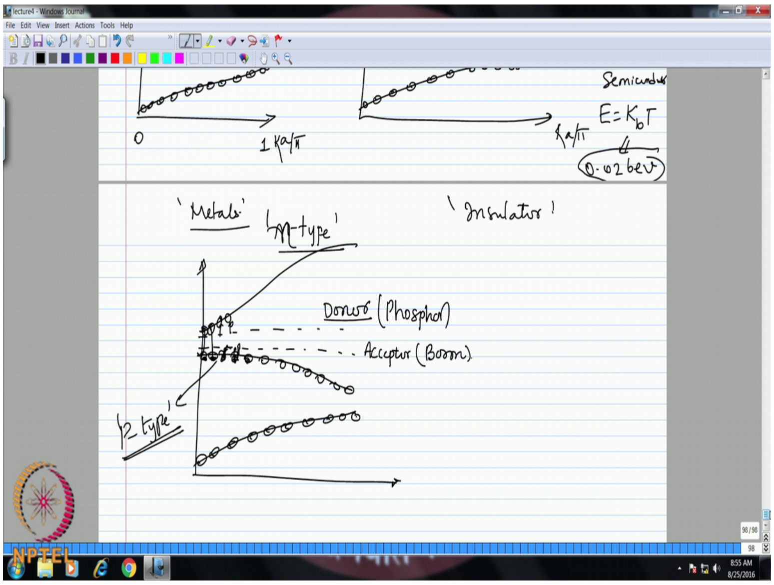

So that means, you take a donor or accepter whose Fermi levels can be tuned to be either close to the valance band of this basic material or to the conduction band. So, accordingly it can become an n type or p type semiconductor.

So, probably you have heard about this kind of explanation when you are talking about semiconductors, but not in terms of the different energy levels and energy gaps. So, if you look at therefore, the n type semiconductor. So, this is all filled now what could happen is this band gap may be OK, to move at certain temperature. So, two electrons may be jumping from here to here and therefore, two holes are created on the valance band, on the conduction band you have two electrons and now you introduce a donor, so the Fermi energy of the donor is basically closer to the conduction band of this material. So, therefore, at higher temperature what will happen? That the chance of these electrons from the donor jumping to the conduction band of the acceptor material. So, these electrons do not have enough energy. So, they cannot simply jump from here to here, but the donor electrons can do because their Fermi levels are closer to be conduction band. So, therefore, this will result in the creation of what is called as n type semiconductors.

So, the donor what, do you remember what is the standard phosphor and what happens when you want to make a p type semiconductor. You want to have an acceptor whose Fermi level will be closer to the valance band of this. So, in this case you call this as acceptor and a commonly used semiconductor is boron on. So, what happens is from the semiconductor material these electrons can jump to the acceptor the energy levels, they cannot jump to their own conduction band, but to the and therefore what happen is, an excessive empty space or holes are created right. So, when these go in the base material you have therefore, holes. So, there this becomes p type semiconductor. So, I mean to give you therefore, a kind of over view. So, depending on the way the energy levels are filled and depending on this forbidden region gap. So, this will decide what is the kind of material it will be whether it is a metal or insulator or semiconductor.

So, this basic understanding is required for you because when you are distinguishing the materials and when you now start looking at calculating all the macro scale or micro scale properties you have to be sensitive to what kind of material you are doing this.

So, we will stop here and from the next class we will focus mainly on these dispersion curves, we will do away with the quantum mechanics. The quantum mechanics in solid state physics is learned only till this point where you know how to produce this dispersion curves and after the dispersion curves are obtain we will continue with that, we will make approximation to the way this dispersion curves look what I have drawn here it could be the actual dispersion curve, but we will make approximation like parabolic approximation and use those parabolic approximations into calculating what is called as density of states. So, we will do that in the next week.

Thank you.