Optoelectronic Material and Devices

Prof. Dr. Deepak Gupta
Department of Materials Science and Engineering
Indian Institute of Technology, Kanpur

Lecture - 8
Effect of Periodic Potential, Origin of Band-gap through Kronig-Penny Model

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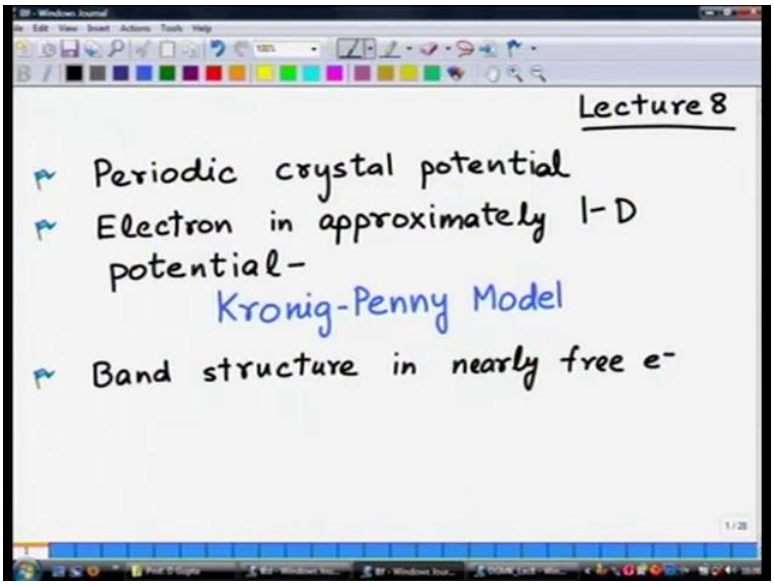

Welcome to lecture number 8. Now, today what we are going to do is, we are going to introduce periodic crystal potential. Actually, we already did say that because of the periodicity in lattice, (( )) the potential which electron experiences should also be periodic. As a consequence of that we did not solve the Schrodinger equation for energy, but we through Bloch theorem we said the solution should be of form the way Bloch theorem gives. And as a consequence of that we showed that there is no unique k vector. In fact 2 k vectors separated by capital K vector, the reciprocal that is vector would yield the same, will give you same, same, same properties.

So, therefore using that concept we are able to show a band confined that k axis of the E K diagram to only the first Brillouin zone successfully. And that was one second thing we said was that the number of k states in first Brillouin zone would be at least the number of primitive cells that are in the that are in the given material. So, those are the two things which I had proved as a consequence of Bloch theorem, because the potential was periodic, but now what we are going to do is that having plotted this E K diagram for free electrons.

That means, energy is taken hypothetically as the free electron energy, but the to show how the x axis, the k axis will be plotted having done that. Now, we need to do improvement on the energy values, and we have to start putting the realistic energy rather than free energy, free electron energy value which are a e by e equal to x square by 2 m k squared instead of that we need to put the realistic energy value.

In order to do that therefore, we must introduce the periodic potential into the Schrodinger equation and start solving it. I have told you that solving a realistic equation in many electron, many body problem is impossible, and we have to reduce it to one electron problem, even when you reduce it to one electron problem. Then you have to consider effective potential, and that effective potential when you start solving then it takes huge computer power to solve that kind of thing suddenly, no identical solutions are possible.

So, what I am going to do is first show the nature of the periodic potential, when I do simple problem I am going to show then this assume then, I will show you the nature of the (( )) here I will show you the nature of the periodic potential. I will assume that nature of periodic potential and I assume that in one dimension only, and viewing 1 dimension only use what is called as Kronig-Penny model. I will show the consequence of this particular potential one dimensional potential, which we are periodic potential, which we apply so that physics physically, we will understand what happens why you see free electrons for metals.

Now, we are interested in semiconductors how does this band-gap originates from when you apply periodic potential is what I will try to show you, from Kronig-Penny model one dimensional so that because it gives me a close form analytical solution having shown that. Then I will assume that somewhere somebody has done the calculation realistic calculations, and then I will start showing them for silicon germanium gallium arsenide and different said conductors in the band diagram.

And since, you know how to read the band diagram so then it will be easy of course. So, today’s lecture is about what is the consequence of and then of course, we will show you the what how the free electron band diagram should be changed, when we introduce this potential in them this periodic potential. So, let us get started with it so let us do it like this, let us look at first an atom. So, suppose I plot the potential so let us say I plot start putting up atom.

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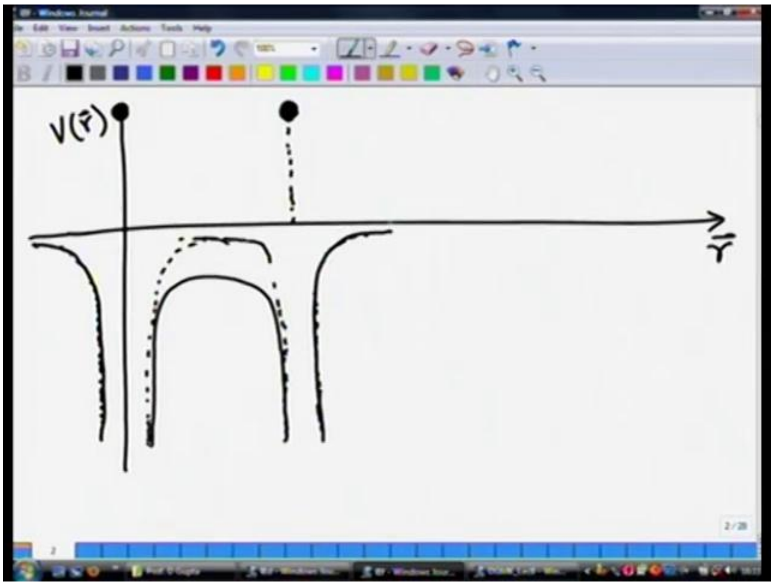

Here is your atom, here is a I am plotting potential so here is position versus let us say here is an atom sitting right here, how does the potential look like I am plotting this as a function of position, potential as a function of position. Then this potential look something like this that as you approach close to it, the potential behaves something like this, something like this. Now, suppose I add one more atom to it at a spacing of certain periodicity with certain periodicity, let me add one more atom right here if I add one more atom what happens?

If I add one more atom then I can plot independently for as if alone there, in that case I will plot something similar for that particular atom like this, that is one into this let us plot this right here. Similarly, I will plot it for this atom also potential for this atom as well something like this and therefore, net potential if I plot would look something like this, for these two atoms is going to look something like. As I add up these two it looks something like this similarly if I plot this for.

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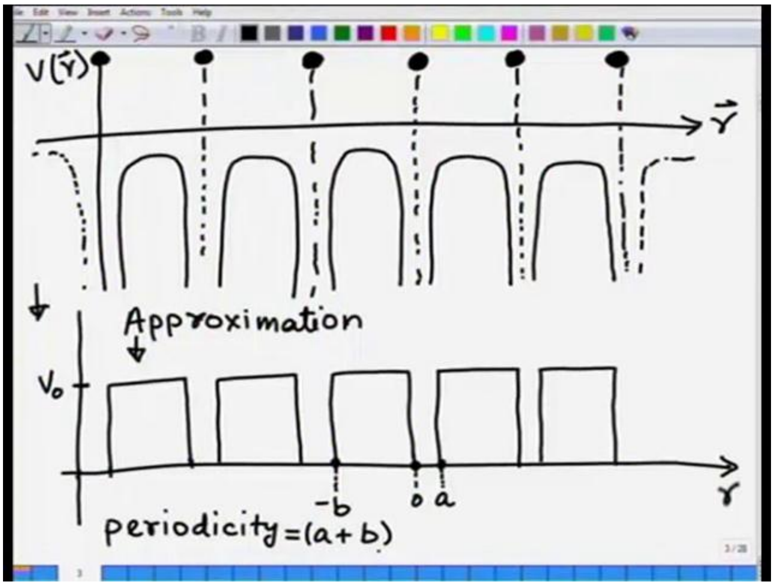

Large number of atoms one dimensional now I am going here is second here is third one here is the fourth one here is the fifth one and so on, this is position and I am plotting other function of addition then I will plot something like this, like this. And as a sum of all these then I will start plotting it potential it looks something like this and so on, and so on. This potential will look start looking something like this, this in our problem. So, this a realistic periodic potential that we have in our one dimension crystal, 3 dimensional crystal will be more complicated than that.

So, effectively what we are going to do is that we are going to reduce in one dimensional approximate periodic potential, I am going to assume this to be something like this so this is the approximation, in order to get a analytical solution. I am going to make a approximation and I am going to make an approximation like this, I am going to make it that this periodic potential varies something like this. I am going to use it square potential or rectangular potential is what I am going to use it as. So, periodicity in this so I am going to use this value as v 0, I am going to use this value as v 0. This is position let us say this is position equal to 0 and let us consider this position to be a, let us consider this position to be minus b right here, right here and right here.

So, these are the positions and these are the periodic potential that means the periodicity is a plus b. So, this is the in order to solve this problem which I just described to you nearly free electron problem, which I want to solve in a periodic potential. What I have done is I have taken a one dimensional lattice, in this one dimensional lattice I have shown how a potential might vary here, how the potential might be periodic.

This periodic potential then I am trying to show you not show you, but going to approximate as a rectangular potential whose value is either v 0 or 0 in the range from 0 to a the value is 0 in the range from minus b to 0 that value is v 0 and this is a periodic potential if imperodicity of a plus b. So, this is what repeats itself. So, essentially Kronig-Penny model is about this, I am going to solve this as a Kronig-Penny model.

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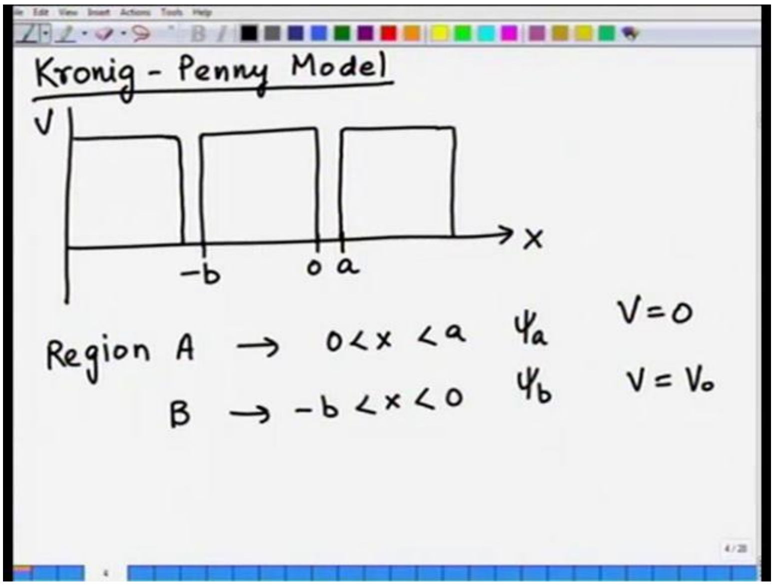

This is what is called as in this solution in this form of potential is called Kronig-Penny model. Which means, that I am going to describe let me re-plot this right here one more time. So, I won't plot it like this. So, I have plot something like this, this is the potential and this is let us now, call this as x direction is to r direction because now this is only 1 dimension something like this, where this is 0 this is a and this is minus b and here is minus b.

And to a region let us call it A, this region A is from x to 0, 0 to a is the region. And region B let us call it that region between minus b to 0, all right? This is the two regions we are going to talk about, in this way the function we are going to call it phi of a in this we are going to follow way function as phi b here, two way function in these two regions which we are going to solve for in this particular problem.

So, what do we have we have again in this case what we are going to do is in this case, we have a in this case potential is potential is equal to 0. In this case potential is equal to v 0 that is the potential in region B and region A. Now, what is the problem at hand, the problem at hand is in this potential we want to solve the Schrodinger equation. So, one dimensional Schrodinger equation so that is the Schrodinger equation, we are going to solve of course, let us write it down now for region A.

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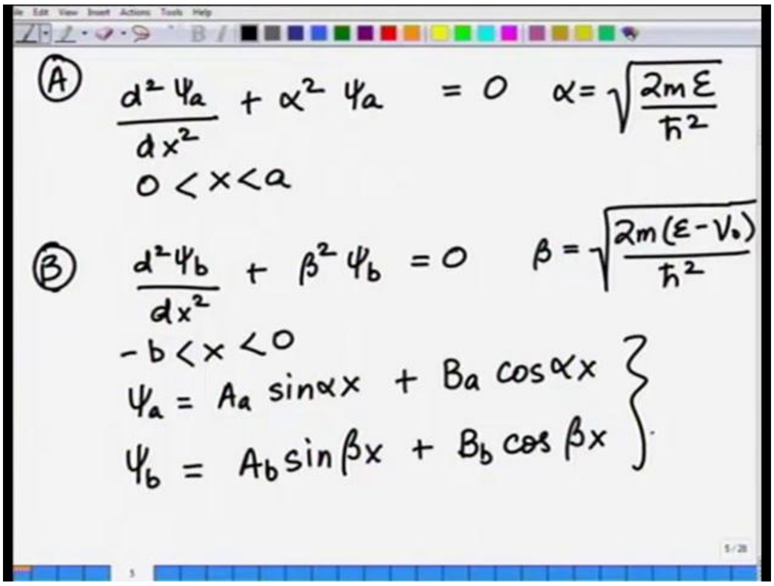

Region A what is the equation, equation will be d square now I can write in so partial derivative because this is all the function of only position 1 dimension x. So, d x square h square by 2 m a in front of it which I am taking in a separate form plus alpha square phi of a of position x by the way is equal to 0. And what is alpha here, alpha is equal to square root of 2 m energy divided by h square. Essentially, in this case v is equal to 0 in this region. In region B I am going to solve the problem phi b divided by d x square plus now, I am going to write beta square phi of b as equal to 0 and this is x equal to a and this beta now is equal to square root of 2 m energy minus v 0 by h square where, now I have x minus b.

So, I have now I am solving in the region this region B, I have essentially a potential v 0. Whereas, potential is equal to 0 in region A. So, I am going to solve these two these two Schrodinger equations together, and apply boundary conditions onto them and to find solution and how the energy behavior would be essentially, that is what we really need to do.

So, I am going to do lot to algebra right now this algebra, I am going to write down here you are welcome to go through the algebra in details, or you can skip the final result whatever you like. I am going to write down the algebra, but when it comes to the solution which becomes important I will point it out, from that point on you must make sure that you understand completely.

Algebra if you wish you can skip, or you can follow completely I am going to write down theoretically. The solution of this equations are of form phi of a should take a form of A of a sin alpha x plus B of a cos alpha x, I am going to write down very quickly on this. So, without too much explanation sin beta x you follow good otherwise skip it, but when it becomes important when you get the start getting solution that is where I will expect that you start following again at least more carefully. So, these are the two forms of solution to these two equations the form is equation is similar to both the equations, where the equation form is same. And therefore, I have written down the solution now we need to apply the boundary conditions.

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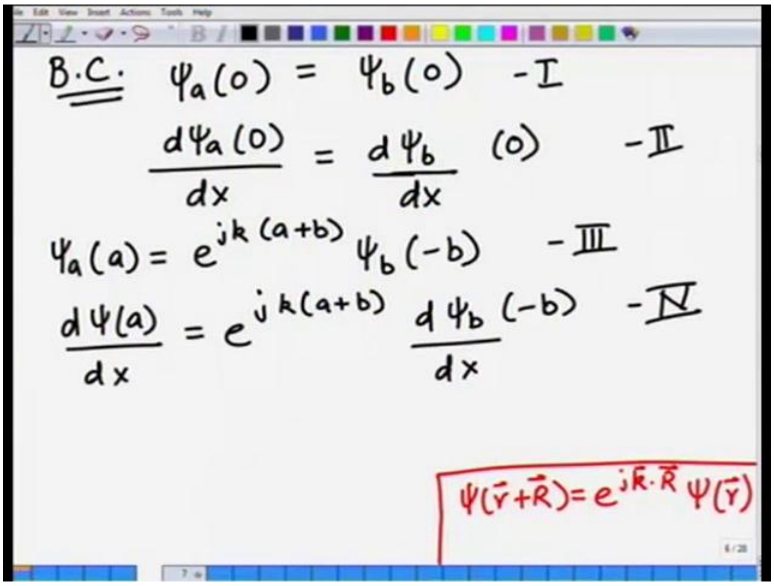

So, these are the boundary conditions which I need to need to apply. What are the boundary conditions at point x equal to 0 at x equal to 0 what happens, phi of a at x equal to 0 should be equal to wave function should be continuous, that is equation number 1 equation number 1. Equation number 2 should be that as you know that for derivatives also be equal to should also be equal that is a requirement on the wave function, that is the nature of the wave function should be continuous at x equal to 0 that is the number 2.

Second as a consequence of periodic potential remember Bloch theorem, which says that periodicity is now since a plus b. So, what I am going to write down here is that phi at the two ends the phase function should defer by phase only, and what is that phase phi of a at a should be equal to e to power that is the phase part j k a plus b that is the periodicity, that is the periodicity in here and phi of b at minus b. We call this is there maybe we can change pen, we call that this is the consequence of phi of r plus R being equal to e to power j k dot R phi per phi of r that is a solution. It can already Bloch theorem, which is what exactly what I have written down here in this case the periodicity is a plus b in this case.

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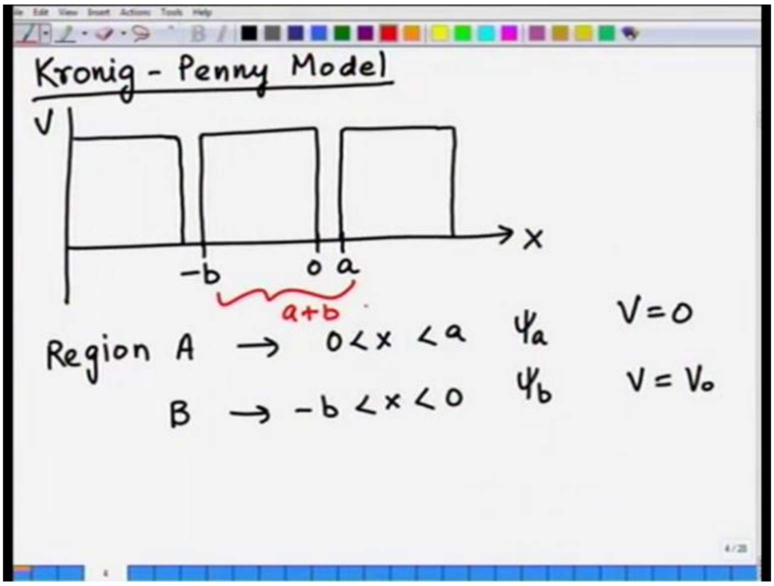

Total periodicity is a plus b is the periodicity here, and likewise the fourth boundary condition is d of phi a at a d x should be equal to e to the power j k a plus b d phi b at minus d of course, at minus b these are the periodic boundary conditions. Consequences of periodic boundary equation number 3 and 4, and number 1 and 2 are the continuity at x x equal to 0. So, these are the four boundary conditions and I have four constants in there which I need to determine possibly, or I have to solve it as characteristic value problem. Eigen value problem is what I may have to call this as. So, let us start applying these boundaries conditions if you start applying these boundary conditions, then from one you will get the 4 equation.

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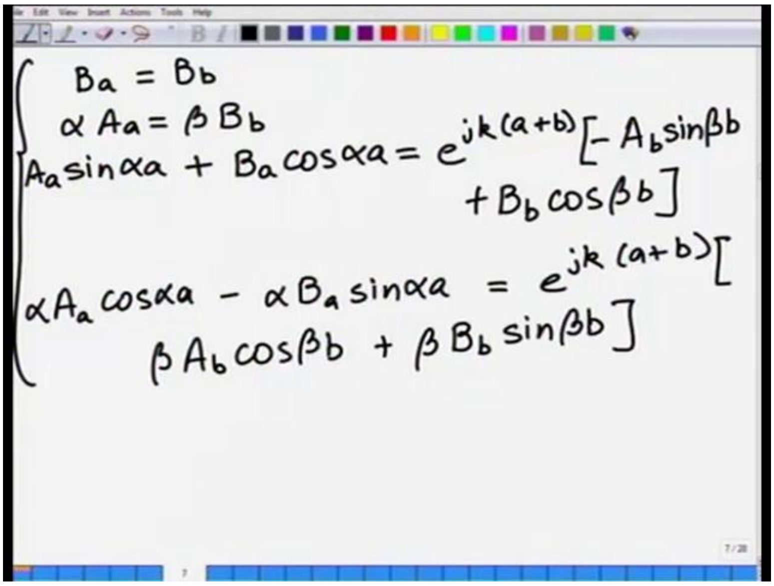

You will get is therefore, B a is equal to B b that is one thing we will get, second is from the second equation we get A a is equal to beta A b. Third equation you are going to get is A a sin alpha a plus B b cos alpha a is equal to e to power j k a plus b minus A of b a b is a constant a of b a b sin beta b plus B b cos. So, these are the our constants are A a B a A b B b. So, we are going to apply this so, let us just correct this equation and there is a here there should b of a here so, that is the correction in here all right.

So, this is third equation, fourth equation will be alpha A of a cos of alpha a minus alpha B of a sin of sin alpha a so be equal to power j k a plus b beta A b cos beta b plus beta B b sin beta b. So, that is these are 4 equations and 4 unknowns, but of course, these are 4 homogenous equations. The 4 homogenous equations they are always have a trivial solution that means A a B a B b and B b A a A a B a, and A b and B b all are 0 is the trivial solution of this. The thing of it is that in fact let us what we want is that in fact if we eliminate.

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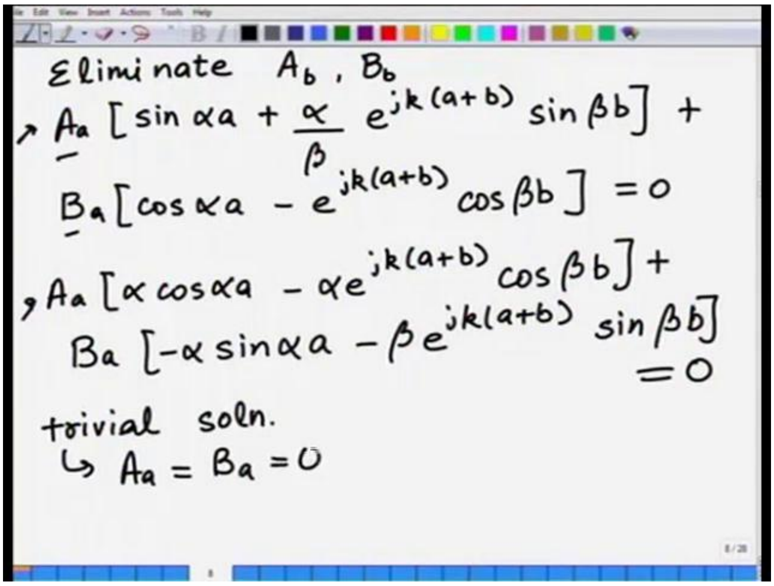

Eliminate let us do one step first and it will get simple a little bit eliminate A b and B and b from these equations to equations and get 2 equations, which are A of a sin alpha a plus alpha divided by beta beta e power j k a plus b bear with me all this algebra, this is just for those students who are interested in completeness. Otherwise solutions will be very interesting that I promise minus e power j k a plus b cos beta b equal to 0.

Similarly, I can write second equation after eliminating 2 variables A as equal to alpha cos alpha a minus alpha e power j k a plus b cos beta b plus B a minus alpha sin alpha a minus beta to the power j k a plus b sin beta b equal to 0. Now, I have instead of 4, I have 2 homogenous equations, in 2 unknowns A a and B a of course, trivial solution is both of these A a and B a is 0, but that is not what we are interested in we are interested in trivial solution is of course. Trivial solution is A a is equal to B a equal to 0.

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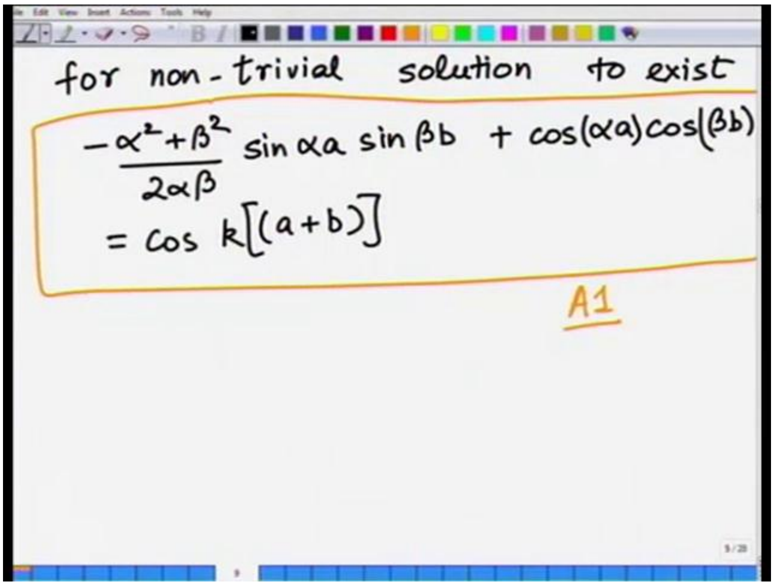

For non trivial solution to trivial solution to exist the condition is the determinant form by the coefficients should be equal to 0. So, if I so that the condition so, in order for non trivial solution to exists. Therefore, essentially that is what it gave this is the condition we are interested in more than solution, we are interested in what the condition of the solution is so the non trivial solution exist, if these 4 coefficients which you see here form a determinant.

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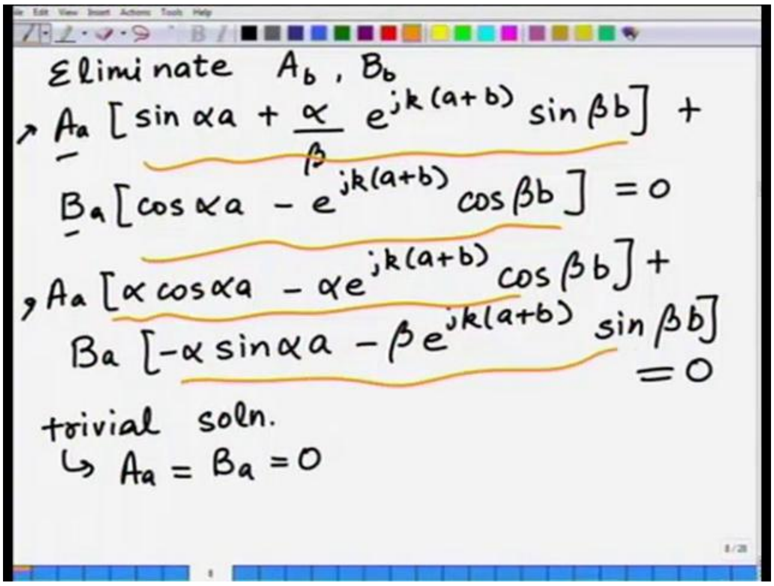

Whose value is 0, so if I write that out and expand its determinant also then I will write this as alpha square plus beta square by 2 alpha beta sin alpha a sin beta b plus cos of alpha a cos of beta b equal to cosine of a plus b. This is really the condition for solution this is essentially what I am looking for, at the end of the day that in order for solution to exist, this must be true that is what as we wanted to show. I am now going to do little bit more simplification let us call this maybe let us give it a A 1, let us call it let us call it A 1 this let us call it new and now solve this problem. Remember now what happens is.

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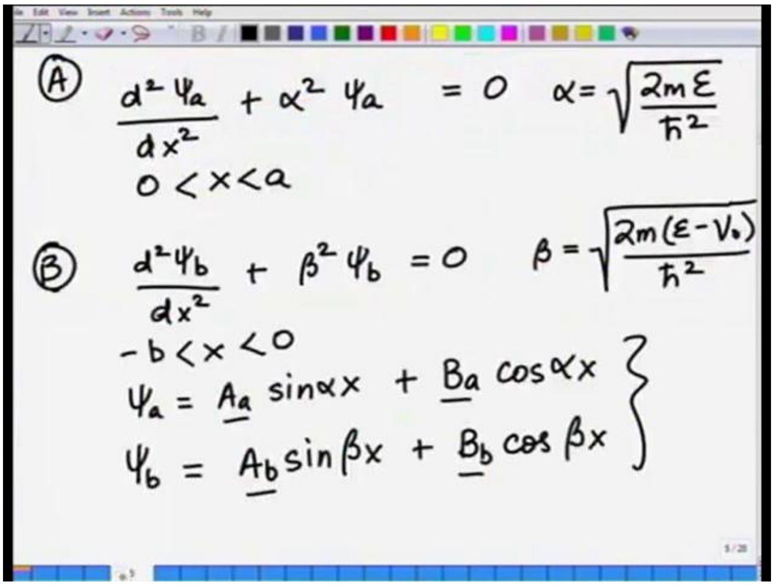

The difficulty we have is this that the solution will takes strain forms depending on the e is greater than v 0, v 0 is greater than e correspondingly this beta could be real or imaginary. Accordingly, the solution may start becoming the solution form a solution will start becoming different. So, we are going to consider these as separate cases, in order to do. So, I am going to separate these out, separate these out by making certain assumptions namely, let us not assumption sorry this modification to how we are going to write it now, what is beta in this so beta is equal to.

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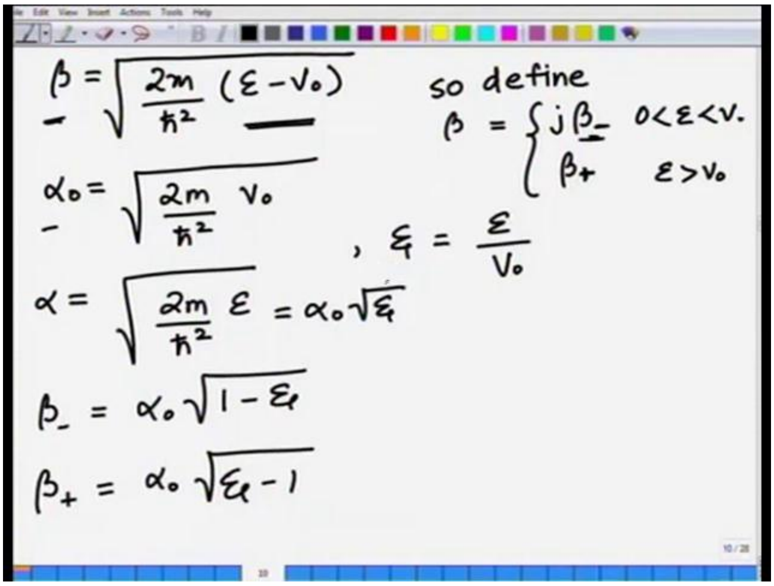

Beta is equal to 2 m by h square energy minus v 0 square root of this whole thing, this is what this quantity is. So, what we are going to define is so define so that we will define beta as equal to j times beta minus or beta plus. So, that both these quantities beta minus or beta plus are always real when this is equal to energy is less than v 0, and when energy is greater than v 0 then of course, beta plus is anyways then we will call beta plus in which case is anyways it is real.

When energy is less than v 0 then beta is imaginary, therefore we exclusively written down that as beta minus so that beta minus is real. Then let us make certain more definitions in there alpha naught, we will define as quantity which is equal to 2 m h square we must in order to give it simply simplify solution. I am making these reduced quantities, I am going to reduce this called zeta, this zeta energy as being ratio of energy to this potential which is in this crystal, so that now what is the alpha?

We call that alpha was equal to we will go back to our page 3 alpha was equal to 2 m energy by h bar square. So, use that so we can now write alpha as equal to therefore, equal to remember that was alpha was 2 m h square energy whole square, this quantity we can write therefore, as alpha square alpha naught times square root of zeta. I can write alpha is like this beta minus as equal to alpha not by same way 1 minus zeta and beta plus as equal to alpha naught zeta minus 1. So, I am now going to use these quantities alpha naught zeta beta minus and beta plus and reduce this equation.

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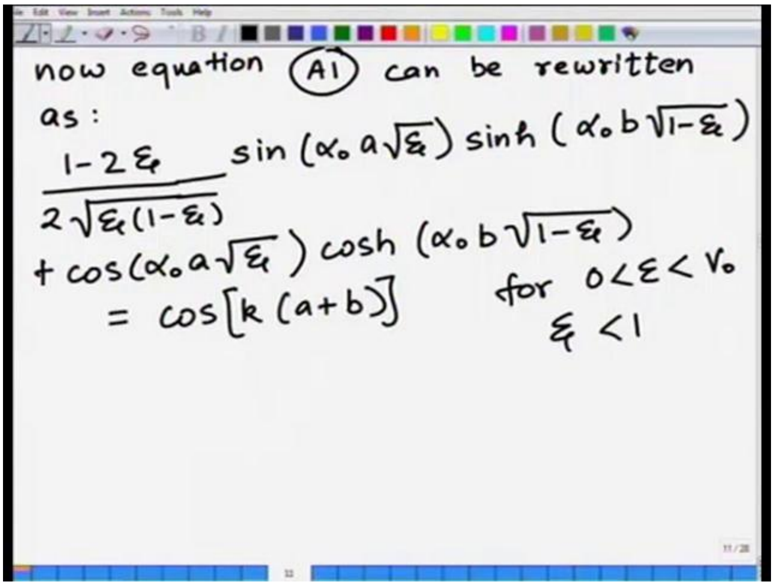

So, now equation that condition of my condition that a solution exists can be can be re-written as, re-written as 1 minus 2. This algebra you can try on your own if you want to, but what is important is that this condition of solution is important. This you must understand that this is the condition, which we obtained from solution of Schrodinger equation.

Now, I am going to process of doing more algebra and writing this in two exclusive forms when, when energy is less than v 0 and when the energy is greater than v 0. That means, when zeta is greater than 1 or when this quantity is greater than 1, or when this quantity is less than 1. So, I am writing down this solution exclusively for two cases so that it is easy to follow so, that every number involved is a real number in that case.

And sin hyperbolic now alpha naught b 1 minus zeta plus cos of alpha naught a square root of zeta cosh hyperbolic alpha naught b 1 minus zeta, and that should be equal to cosine of k a plus b for when condition when energy is less than v 0. That means, zeta is less than 1 these are the condition, and this is a hyperbolic function is we are using in here. The hyperbolic appears because now this beta will be an imaginary quantity.

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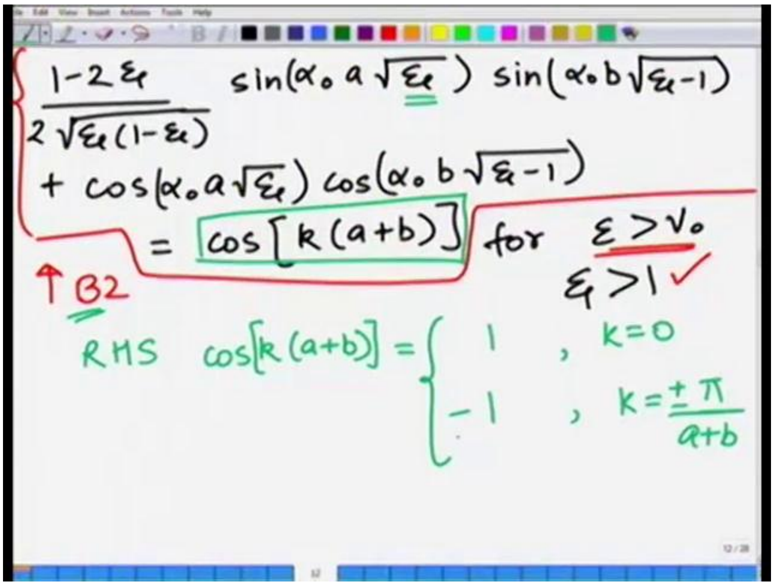

Similarly, I can write 2 similarly, I can write this as 2 zeta 1 minus zeta sin of alpha naught a zeta sin of alpha naught b zeta minus 1 plus cos of alpha naught a zeta no hyperbolic cosines. Now, because hyperbolic cosine and cosine now because every quantity in the since energy now is greater than v 0. Therefore, this zeta is greater than 1 for that condition, I am writing now the equation in that case simply A 1 all the quantities of A 1 in any case were real.

So therefore, in equation A 1 were real and therefore, beta was real and hence we do not have any hyperbolic functions here. So, cosine of alpha naught b square root of theta minus 1 and that quantity should be equal to cosine of k a plus b and this of course, for as I mentioned energy greater than v 0 and zeta therefore, greater than 1 that is the condition.

So, that is the let us call it as let us call this equation as if you wish B 1 and let us call this equation as B 2. So, B 1 and B 2 are these equation now, which we are referring to and this is this is the condition for solution to exist, when zeta is less than 1. That means, when energy is less than 0 this is the condition of condition for solution to exist, when energy is greater than or e energy is greater than v 0 and that means, zeta is greater than 1 for all those conditions. Now, we are going to explore what this solution means, as a consequence solution, what happens is what we want to explore now.

So, let us try to do this what we are going to do is, we are going to plot this left hand side. So, we are going to plot this left hand side for these two functions together. That means, we are going to plot we are going to plot this left as a function of zeta, as a function of this quantity zeta we are going to plot the value of left hand side. When of course, zeta is less than 1, we will use this equation B 1 when zeta is greater than 1, then in that case we will use equation B 2. And then according therefore, we will plot this left hand side of these 2 equations as a function of zeta, so let us do that.

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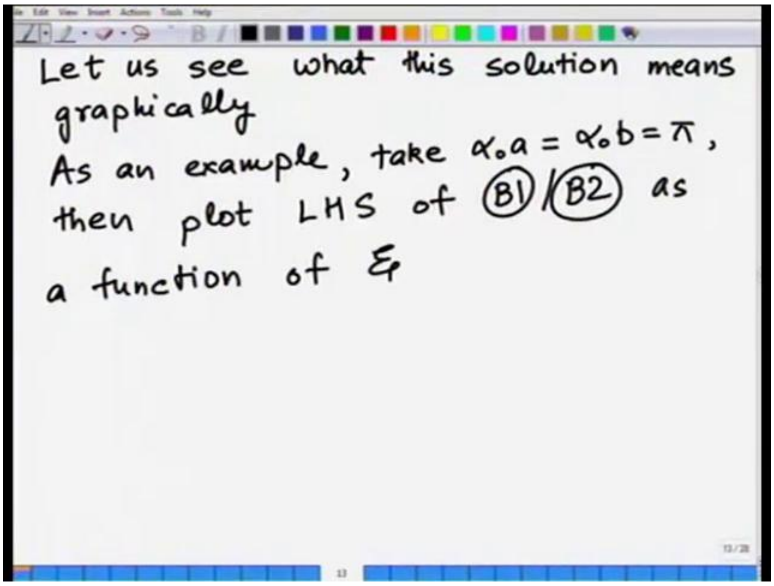

Let us let us see what this solution means graphically, as an example as an example take alpha naught a equal to alpha naught b equal to pi. Then plot B 1 slash B 2 equations B 1, L H S left hand side of B 1 of B 1 and B 2 as a function of zeta, let us see what happens to this. So, let us do this plot so, what I am going to do is.

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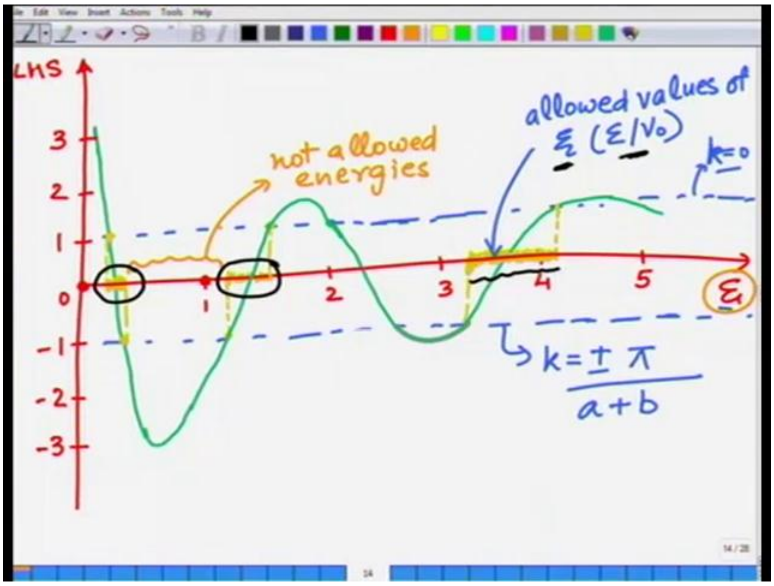

Then here my big axis here this axis is running here, this is zeta and let us say this is 1, let us say this is 2, let us say this is 3, 4 and this is 5. So, when zeta varies from 0 to this point 1, we use B 1 equation and for all points beyond 1 we use B 2 equation. And now I am plotting, left hand side for this condition for these values taken here, let us plot this 0, 1, 2, 3 minus 1 minus 2 minus 3. So, let us this plot this function use the different color pen now, and what I am going to do is I will put some markers on this also, I am going to put this marker here and when this left hand side is equal to plus 1. And when this side is equal to minus 1 this are two markers on this putting for our sake here.

Now, let us start plotting this so this let me see I want to pass through which points, that is what I want to make sure that I do not. So, this curve goes something like this and I plot this left hand side it looks something approximately like this let be above value say like this. So, this curve looks something like this. Now, let us go back and look at these equations. So, this a plot of left hand side, but what is the left hand side when does the solution exist? Solution exist only when left hand side is within the bounds of minus 1 and plus 1.

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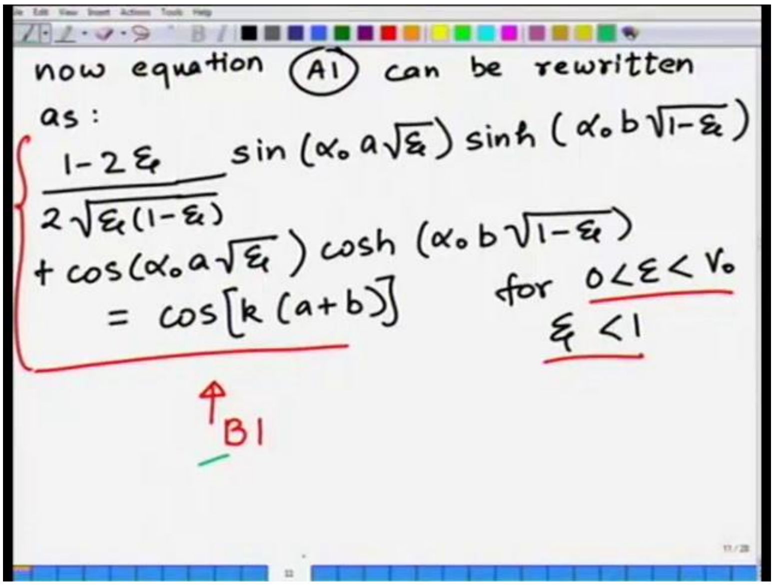

Since, right hand side is bounded by within sin function and is real is bounded between minus 1 and plus 1 solution will exist, only if these values of left hand side are within plus 1 and minus 1, all values outside beyond plus 1 and cell minus 1 will not satisfy this equation. Now, so this right hand side since, it is bound between plus 1 and minus 1 therefore, that the solution will exists only when left hand side, which we have just plotted is also within plus 1 and minus 1 then only solution can exists.

What is that means, this let us quickly then write down write down that inside if you look at the right hand side in this case. So, cosine k a plus b is equal to when k is equal to 0, this is equal to this is equal to this function is equal to 1, and for k equal to plus minus pi divided by a plus b this would be equal to minus 1, this function will be equal to minus one for this condition.

So, that is what this will be so essentially therefore, I can write now that this value therefore, corresponds to so this bound, which I am showing you is for k equal to 0, when k is equal to 0 at k equal to 0 this value plus 1, and of k equal to plus minus pi a divided by b that periodicity, so that is where value of right inside becomes minus 1. Essentially, whenever this dream function this green curve is when green curve is within these 2 blue lines then only the solution exists. So, let us look at this solution that means, the allowed values of this quantity zeta allowed value of this zeta must lie between here and here.

So, this must be the allowed values of corresponding to this and corresponding to this, this must be the allowed values of zeta this must be the allowed values of zeta. Similarly, corresponding to this and corresponding to this from here to here should be the allowed value of zeta. Otherwise, beyond this zeta you cannot have values of zeta beyond this because this function goes beyond either plus 1 or minus 1.

Similarly, you could have in this range your value is allowed zeta is these what we are seeing the blue line, this yellow lines yellow portion of it this is where therefore, allowed values of zeta. We should remember this energy divided by v 0, these are essentially therefore, allowed (( )) of energy. Now, you see beautiful results there is that what do you notice in here now, we see origin of band gap. That means, now we have allowed here we have allowed energies, we have allowed energy, but in between our energies is not allowed, not allowed energies in between we have so that is now, first time we have seen that metals had no band gap, free electron theory could possibly described them.

Now, we can we can see when we introduce realistic when you start introducing periodic potential not realistic yet with approximate periodic potential, then you can see the band gap begins to emerge, and that is what is a characteristics of a semiconductor. So, I wanted to show you the what the origin, origin of band gap is and what is where does this band gap happens. The band gap happens at the edges of the broiling zone and k is equal to 0, this is the Brillouin zone where is the Brillouin zone.

Remember for one dimensional lattice I had shown you the Brillouin zone goes from minus pi by a to plus pi by a, but in that problem a was the periodicity of that of that one dimensional lattice. Now, in our case the periodicity of one dimensional lattice a plus b therefore, my Brillouin zone goes from minus pi by a plus b to plus a plus pi by b and which is this point.

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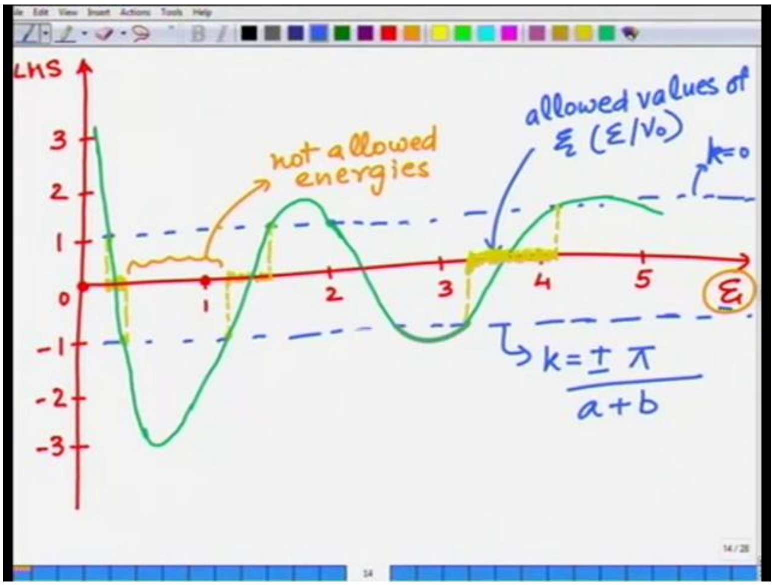

So, you can see that at something happens at edges of Brillouin zone and also were k is equal to 0. That means, at the lattice point themselves also something happens reciprocal lattice points also, something happens, something happens and around that point a values of not allowed energies begin to appear. So, let us make let us quickly make some observations, what do you see.

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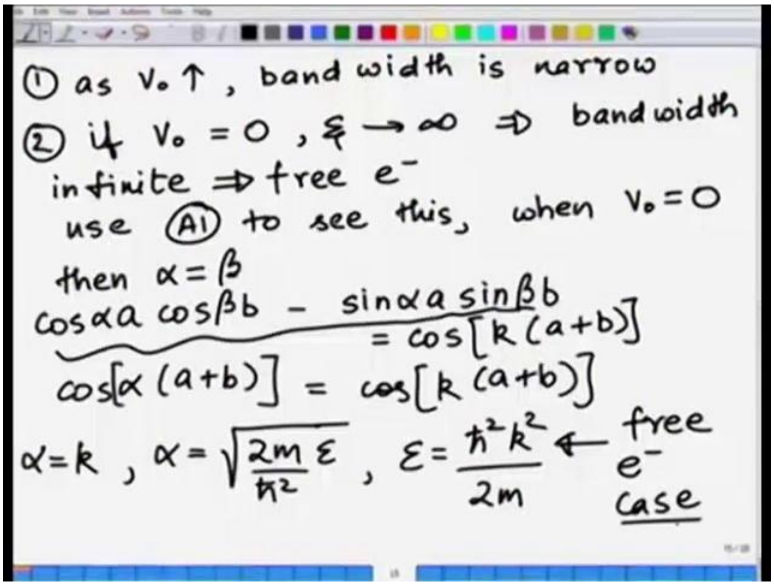

One as v 0 increases as v 0 increases means, what notice v 0 increases means, zeta becomes small and small v 0 increases means, zeta becomes small and small that means the on the left hand side. In that case band width is narrow, what does that mean? That means, notice this particular band it has small width allow value of energies, or zeta allow value of energy has small range compared to this which is wider, which is at a smaller as greater zeta. That means, smaller v 0 and this is even larger width of the band allowed energy is that is allowed energy is even bigger, even bigger range.

That means, the band width becomes narrow and narrow as v 0 increases that means they are moving towards zeta smaller and smaller zeta. And conversely of course, as v 0 decreases therefore, or energy then the band width becomes large and large, which you can visualize that if I have a small potential then until I cross that potential. Once I cross, once I have the kinetic energy, once I have total energy is much, much greater than the v 0 then it will be like the free electron it will not see the potential, but when I am coming close to that potential I will see different band width.

And as I am going deep into the putting potential deep into potential well in that case, my band widths will become narrow and narrow to the extent that they will become discrete, which we will see. Now, second you can see if v 0 is equal to 0 if v 0 is equal to 0, then what would you notice. Graphically, you can see that v 0 0 is free electron that means, all values of energy allowed continuous band.

Now, you can see v is equal to 0 means zeta is tending to an infinity and since, you can notice that as you go higher and higher zeta, the bandwidth becomes larger and larger you can assume. Therefore, you can see graphically in the sense graphically that as zeta will tend to infinity, this bandwidth will also become infinite. That means, it will become a continuous allowed set of energies so, that is something you should be able to see that is zeta tends to infinity in that case bandwidth implies bandwidth is in infinite is infinite.

And that is the case of free electron as we expected, that is the case of free electron as we expected. So, then as if possible if you wish we can go back to our equation this A 1 equation, which we have written down and you can substitute in there for the case we are dealing with namely, when alpha is beta. So, if we take alpha equal to beta and substitute v 0 equal to 0 in their v 0, v 0 in equal to 0, sorry v 0 equal to 0 means that alpha equals to beta. So, we substituted in their this quantity then how would this equation look like, let us do that quickly maybe use A 1 equation to see this, see this that is when v 0 is equal to 0 then alpha is equal to beta.

Remember alpha beta difference is the energy minus v 0 since, 0 is 0 for alpha should become equal to beta in that case, this I can write this A 1 equation as cos of alpha a cos of beta b minus remember let us go back again so, to that equation alpha is equal to beta. So, alpha is equal to beta. So, this will full this will cancel out in the what is in the front and therefore, I am writing this cos of alpha a cos of beta b minus sin of alpha a sin of beta b should be equal to cosine of k a plus b it is what it should mean.

That means, if I look at this then this quantity is cos of what alpha a plus b cos of alpha a plus b cos of k a plus b. What is that mean? That means, alpha is equal to k and that means energy, and what is alpha is definition of alpha is remember 2 m by h by square energy. Since, alpha is equal to k therefore, I can now write alpha is equal to h square 2 m k square which is what the free electron case was, free electron case. That is what the free electron case was so, we can clearly show mathematically also, and graphically we can see also. Similarly, you can do third case also if v 0 tends to infinity that means, you have infinite potential very, very large potential in that case.

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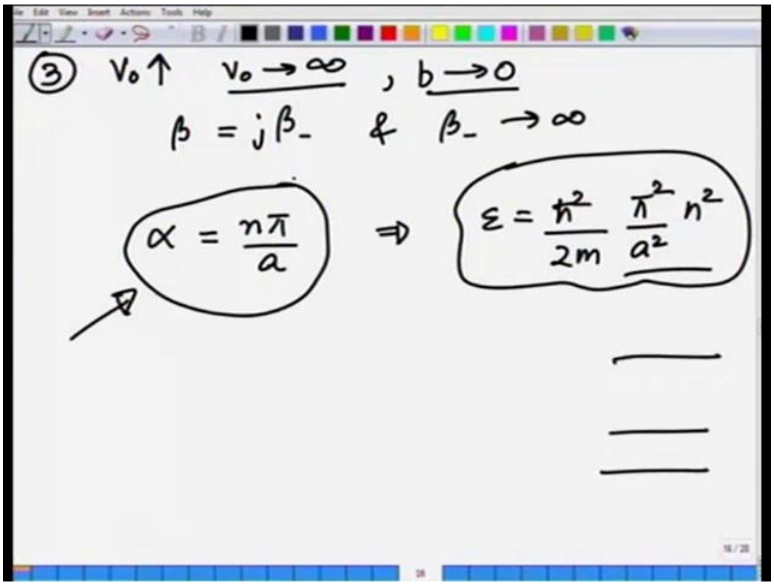

That means v 0 tends to infinity in order to have a finite strength simultaneously, we will ask we will, ask this question that is that if this v 0 which I am plotting here. It should have been v 0 here I can see v 0. So, this is v 0 this quantity is v 0 right here this v 0 when this v 0 is going to infinity then simultaneously, we are going to demand that this width, this width b is also very, very thin almost tending to 0 then only this can be analyzed. And simultaneously, we are going to ask that b goes to 0 if you use these expressions then now, you can see that beta will go to j beta minus and beta minus will go towards infinity in this case.

You can check this out, and if you work through it you can show that in this case that alpha in this case, alpha I am not going to go through the whole thing, but alpha you will be able to show will be equal to n pi by a, which then says that energy is equal to h square by 2 m pi square by a square n square. Remember that is a discrete energy levels, like a hydrogen atom, like in a hydrogen atom the discrete energy levels particle in a box problems will be covered from this itself, try this out yourself this approximation consider this as an assignment part.

As to how to prove that this energy is equal to this quantity right here. As I have shown here when v 0 goes to infinity and v goes to 0 in that case try finding. That means of course, v 0 goes to infinity means zeta goes towards 0. So, use equation A 1 to see if you can simplify to this energy, if you can simplify alpha is equal to look at this quantity you will get your solution, we will get this answer.

So, this are few observations which can be made in here as to what the behavior of so really striking results, we are seeing that if you use periodic potential of course, it recovers back when v 0 0 will be covered back near free electron theory. When v 0 is 0 v 0 is infinity then we start looking at particle in a box like solution that means, discrete energy levels. And in between for all intermediate values of potential in that case, we start seeing that now is the consequence of periodic potential near k is equal to 0. That means, reciprocal lattice point, and Brillouin zone we start seeing a discontinuity disallowed values of energy. So, now what do we do now how do we represent the band diagram. So, approximately…

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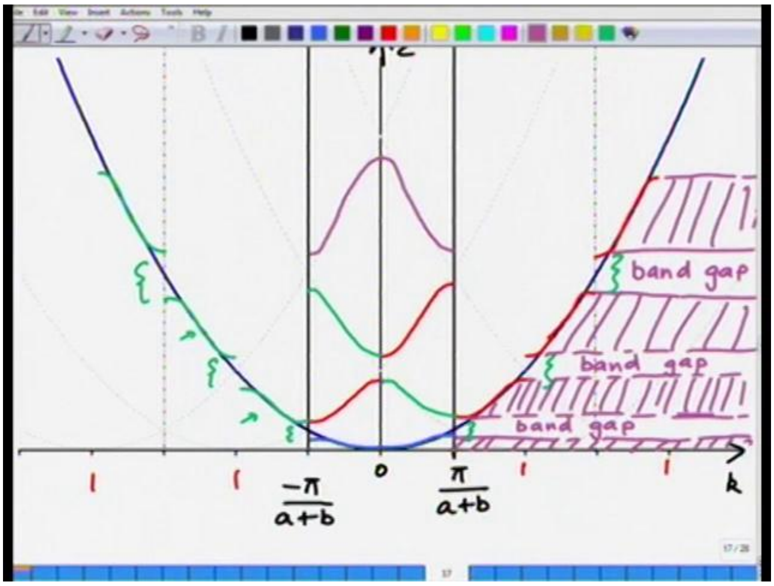

Therefore, will represent the same band as follows now, let us attempt it again one more time. This is k and this is energy we are plotting energy we are plotting and now, we are plotting energy as we derived from Kronig-Penny model. So, now this quantity should be pi divided by a plus b that is the Brillouin zone minus pi a plus b rather, than a because periodicity now is a plus b. So, do not get confused about that and this is 0 this is k equal to 0 is this point and now, what happens we know that something happens at edges of Brillouin zone remember at I had shown you.

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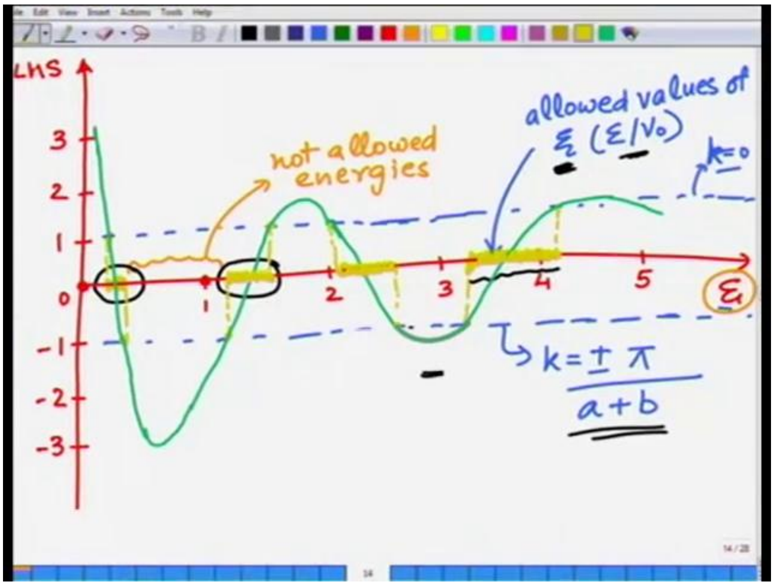

That at plus and pi plus minus plus minus pi a plus b right here we are going to go out of this left hand side will go out of minus 1 and hence, though this disallow values of energies those values will become... I have to in this figure I should also show you that there were some more the other band which I had missed here, which is right here. So, we can allow the value of energy, which I missed earlier plus used this also, here is a allowed value of energy this in here as well in between.

So, between these two values band gap emerges at these values when it goes beyond minus 1. So, I am using this idea to show something what we do is so then simply show this curve as follows. So, near the band edge something happens and we want to show this by showing it curve this like this, in this form. And what else has happens correspondingly remember that red line we had we got correspondingly, we going to show here like this, this curve will remain like this and we will show like this.

And since, something happens also at this k point when k equal to 0 that means, the reciprocal that is point this is reciprocal lattice point, and here is a reciprocal lattice point, here is a reciprocal lattice point, here is a reciprocal lattice point, here is a reciprocal lattice point, here I have marked this points out. So, at this point since against what I am going to do is show this in the same way showing that it is almost free electron like a free electron except that the special points, this curve changes it shape and so on.

Likewise I had shown you for green one, I used a green color also I am going to use the same color here also and we are going to show it like this. We will show this part of curve like this say showing that there is a origin of band gap here, near these points there a band gap opens up, this is what all we show as nearly free electron. And these are the band gaps opening up is what we are trying to show here.

Now, if I plot the same these energies becoming now Kronig-Penny model energies. So, instead of using free electron energies, we translate them back into the first Brillouin zone which is what we always wanted to do, or which we which I showed you for free electron theory also. Then the way we would plot this is then this red line would now, transform into somewhere red portion of the curve will now, transform like this. The red portion will get transformed in this falling fashion, and the green portion will then this particular segment will get transform in the following form.

And this particular segment will get translated in the form where it is like this, and if we continue on this then similarly, we would have so next one could be then like this, coming out like this. And in the first Brillouin zone therefore, showing you that there is these are the allowed values of energy. So, this right here this is the allowed value of energy then there is this, allowed value of energy then there is this, allowed value of energy these are allowed values of energies then similarly, from here onto somewhere here is allowed value use of energy. And these are in between the band gaps, these are the band gap.

So, what I have done hopefully is shown you right here we have another band gap, band gap. What I have shown you is as a consequence of periodic potential therefore, what I have been able to hopefully we will convey to you that the band gap emerges, and in this particular Kronig-Penny model. The band gap is emerging near the Brillouin zone remember that is where the electrons wave is strongly reflected, consequence of that this band gap emerges though, we would not get into the physics of how much this quantity will be. And what precisely happens, but you get the idea that this semiconductors are because of this periodic potential into the lattice into this, in a the periodic potential that is inherent in the crystal having done.

Therefore, having shown you the energies which are somewhat better energies than the free electron energies, and this is a closed form solution I could give you in order to show to you that what the consequence of periodic potential will be one dimensional I made the approximation. And second approximation I made was the nature of the this rectangular periodic potential based on that we could identical solution, on this identical solution based this is I could how you the band gap emerges, but from now on we will start using calculated values available in literature, in text books.

We use those literature values and put it on the band diagram, those energies in band diagram and then our nature of band diagram would be more precise as it should be. Which I will start showing you from and tend like a from one lecture past next not next lecture, but one after that. In next lecture now, what I will do is given the band diagram has this kind of behavior here what does E K diagram, within the first Brillouin zone itself can give you.

What information can it give you, can it tell you about electron velocity, can it tell you about the effective mass, what is effective mass, what is velocity of electron, what is acceleration, what is momentum of can you do dynamics of electron by looking at it. And how does optical properties, how do you interpret optical properties from this band diagrams. Now, those are the things we will start discussing in the next lecture, before we start showing the real diagram and start interpreting, which is a good optoelectronic materials and which one is not. So, before I end this lecture let me also just give the finishing touches. Now, just quickly look at this so, what happened?

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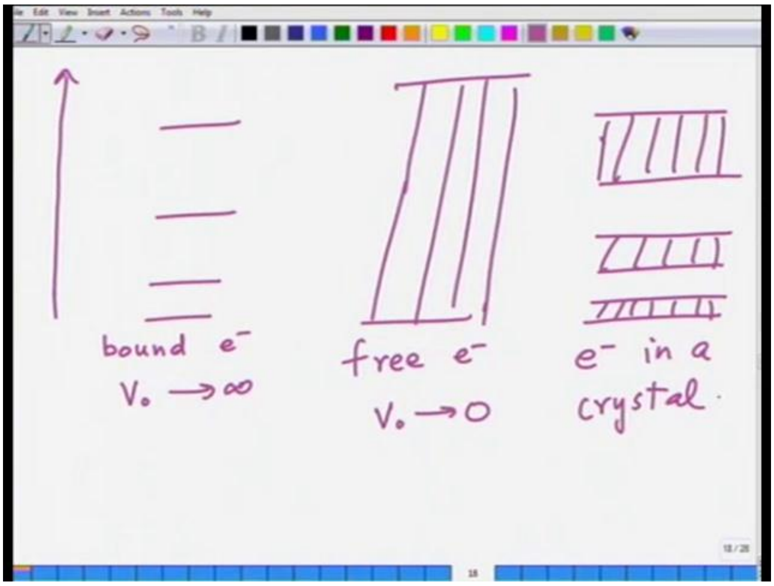

Let us summarize this if this is energy, this is the energy axis then what happened we got solutions which are like this. Discrete energy levels, there this discrete energy levels we had allowed energy levels bound electron, bound electron when we said v 0 goes to infinity that is what we had in this case. Second case was that free electron that means, all energies were allowed, all energies were allowed, there was a free electron free electron when v 0 was going to 0. Intermediate what we had was like this, allowed energies a gap, allowed energies a gap, allowed energies extra. This is electron in a crystal that means, periodic potential which I could show a differently.

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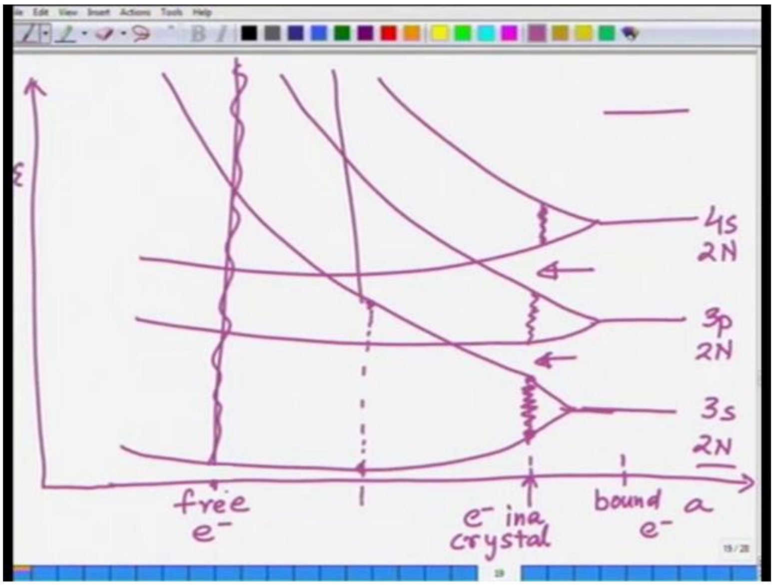

This energy versus imagine like this that this is think of this as lattice parameter, or inter atomic distance. What happens to this energy? Now, energy remember when atoms are far, far let us say silicon atoms copper atoms are far, far apart then what happens they behave separately. So, I have these energies levels this discrete energy level therefore, so I have all these discrete energy levels like this, let us say this is we could give a name as 3 s, 3 p, 4 s extra, extra you can give all these names to them.

Suppose, the N such atoms then I have 2 N electron in each of these, 2 N electrons in each of these levels. And there are all sitting on same energy levels because they are not interacting electron atoms and their parts are apart. Now, start bringing them close as you begin bring them close, what happens to the electrons in this levels? Now, since they start interacting. So, this energy levels will start splitting, if in this case suppose the smallest energy level at this position, when they are so close to each other at this distance close to each other, this is the smallest energy of these electrons N electrons of 2 N electrons.

Now, start splitting into energy and I start getting huge range of all these different energy allowed energy ranges, allow we different energies which are available in this split this is the highest and this is the lowest. So, if I plot only the if I plot only the what is the lowest and the highest energy available. That means, this is at any given a this is the energy range in which all these energy levels split up, then if I do so for all these if I do so all these, what do you notice?

You notice that somewhere at this case then I have these are the allowed energies, these are the allowed energies, these are the allowed energies at this a value at this a value and the situation of bound electron. At this situation we have electrons in a crystal namely, these are the allowed energies and there is a gap, and that there is a gap in here in energy. Whereas, as I move here somewhere here in here in this region this is free electron, all values of energies are allowed all values of energies become allowed, there is no gap in this case. So, you can visualize and physically that is why the band gap emerges with this let me close the lecture.

Thank you.