Optoelectronic Materials and Devices

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Module - 01
Lecture - 06
Electrons in a crystal, Bloch's electron

So, welcome to lecture number 6. So, in this lecture now we are going to start putting electrons in a crystal and I will talk about Bloch's electron. So, we are still building our base how to represent e versus k diagram. So, if you recall that we just did last lecture we did reciprocal that lattices, last two lectures we did reciprocal lattices. Idea was that of course, that electron wave which had a small cave that in their vector its dimension was in a reciprocal space.

Then we generated capital k vectors, those reciprocal lattice vectors, those are done with the purpose, those vectors we are going to use to represent the ban band diagram that is e versus k diagrams. So, ultimately we are going to be using that, but still we are building towards it. So, what I am going to do is remember, now I am going to start including the crystal crystal under lying a.

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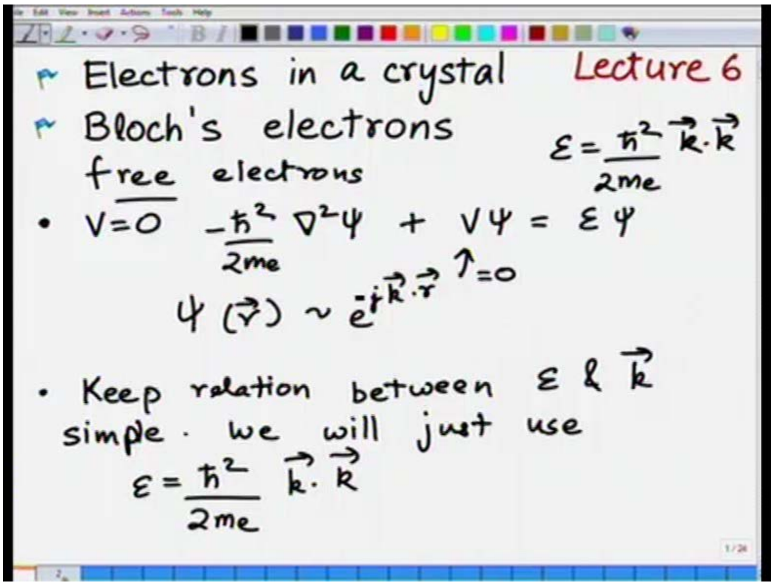

So, far we did free electrons, that we started with free electrons. In free electrons what we did, what are the things we did, let us think about the free electrons? When we did with free electrons, in this case what we did was two things we did. First we said this all this electrons are non interacting, neither their was a ion in electron interaction nor their was electron electron interaction. Therefore, we did this V is equal to 0 is first thing we did in our solving our (( )) the equation which was this h square by 2 m e. In this equation we had substituted V is equal to 0, we had made this go away, we had made this quantity equal to 0 and we had made this go away.

Then we said this is free electron and what did we get? We got energy as equal to h square by 2 m e k dot k or k square is what we got, that is what we have derived for a free electron energy. Now, here comes problem ok fine, saw that it does a improvement it gives us some better result then Drude's theory. But then we also said that many things free electron theory does not explain, it does not show why should a material should be a insulator? Why material should be semi conductor? It does not show, for example, why an aluminum the hall coefficient should be of opposite sign than expected, etcetera, there are failures of free electron theory which we discussed.

So, what we need to do we said, that we will have to include these electrons, what we have not done is that we have not we have ignored the underlined lattice, its periodicity etc. So, what we have to not do as a improvement do is we will solve the problem in two in two steps. In first step what we are going to do is that we are going to keep keep relation between e and k simple, we will just use the result of free electron theory that is e is equal to h square by 2 m e k small k dot small k which is a vector. Of course, in this case in this case the solution we got was phi was of position was e to power minus j k dot r that was in formula solution we got for this. So, we will continue to use that as solution in there.

Now, so first step we are going do that, second step we will include, we will include the potential, we will include the include the potential which will or may be present. Now, what is that mean, just look at it, what is the potential mean? Well where is potential come from? Now, imagine V comes from what? It comes from you can see that many, many electrons, there are many, many electrons in the system. Let us divide electrons we can think of valence electrons, we can think of core electrons, we can think of nuclei. So, in a crystal in a crystal we will have interactions between valance electrons, we will have interaction between all these entities nuclei, so and we have many, many electrons.

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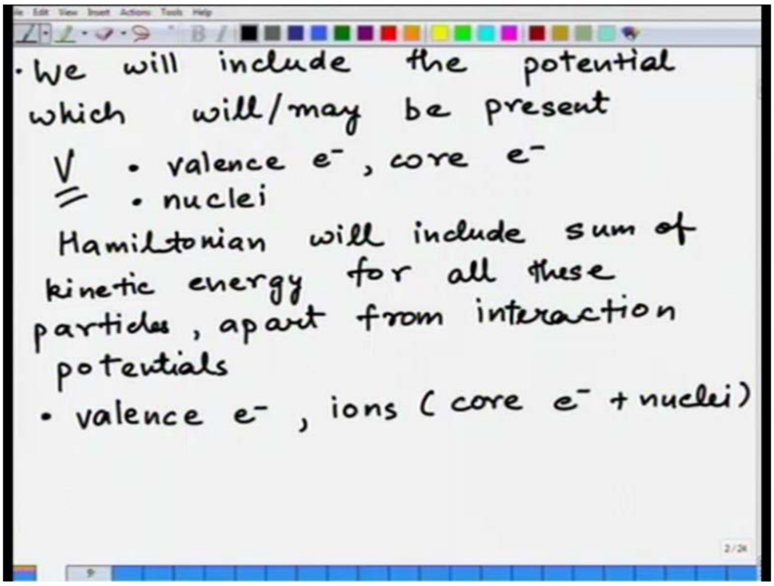

All the electrons, all the ions, all the nuclei which are present in their in the system, all these are interacting with each other. In dead we can write a potential for it, so if were to (( )) solving the equation for it, then we will have the Hamiltanian will include some of kinetic energy I should say. Energy for all these particles, kinetic energy for all these particles apart from potential, that in dead would be of a really formatable problem and to date there is no way of solving such a problem. So, first the approximation we make is we think of valance electron and ions which means core electrons plus the nuclei.

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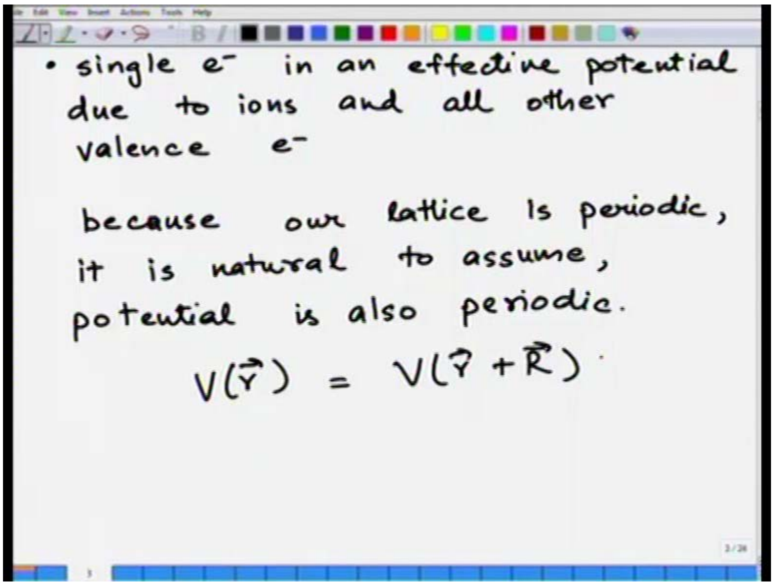

So, that all is bared, the core electrons get bared with nuclei and we call them ions, that is one thing first. But still we have huge number of valence electrons and we have huge number of ions all of them all of them are present still the Hamiltanian include kinetic energies, because all these entities and again the potential. Essentially then what is done is that this problem is still remains formattable and impossible to solve with the present day computers. So, what can you do?

So, one way is certain ingenious formulation made in which you consider a single electron problem, you reduce the whole problem, if you have equivalent problem which has single electron in an effective potential. In an effective potential due to ions and all other valence electrons, that to all other valence electrons. So, that is what we are going to have all other valence electrons and ions will then will reduce that will in effective potential the engineers formulation for it. So, that you treat the single electron you solve the single electron showed showed in the equation in a effective potential.

Exact solution of this problem is beyond the scope of this course, so what we are going to do interested in is we will assume what the result will come out of this. But we are going to do interested in is that notice because because our lattice is periodic, it is natural to assume potential is also periodic with same periodicity. Since, the period in the lattice is capital R therefore potential at any position must be same as potential, it should also have periodicity of lattice which is capital R. So, that should always be true. Now what we are going to do is solve this whole problem in two parts.

First we are going to look at the first part which is going to start now is not really solve the problem. I am going to use this energy relation is the same e is equal to h square by 2 m k square, that means whatever we got from free electron theory, let us keep the energy relation same. Then what are we going to say is that what is the consequence of the fact that underline potential is periodicity been shown here. So, if this is the periodicity then what will be the consequence on. And how can we use that to represent the band diagram and energy will be used in as electron energy. But using this idea of periodicity of lattice and therefore that of potential, how can you represent energy versus k diagram, that is really we want to do. So, let me try this one more time.

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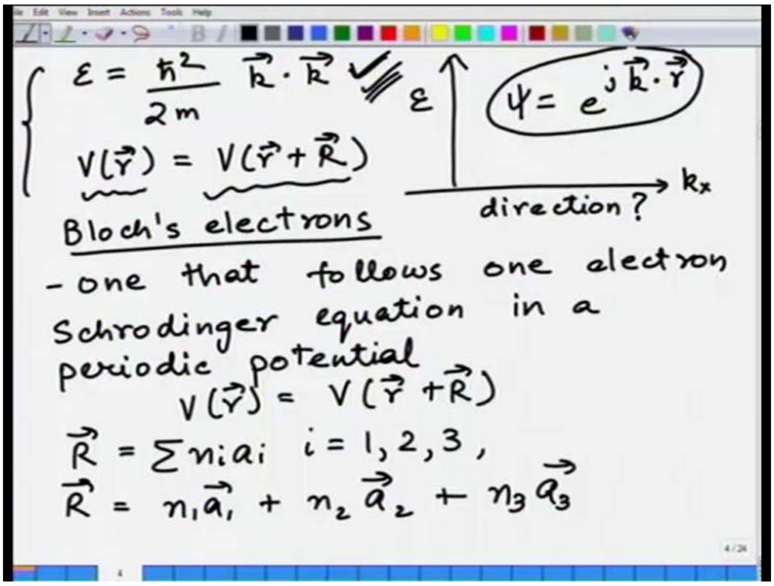

So, energy we are going to assume as h square by 2 m k dot k, now you can already appreciate what the problem is. Problem is my paper is two dimensional, if I want to choose right this energy versus k diagram is what I want to make. What since k is vector, so it has infinite possibilities it could be pointing any possible direction, which direction should I represent here, direction should be what, what vector should I take? That is my problem. You see we can pick only one particular direction, let us say pick only one direction called k x for example, if you pick this k x direction then that is only one equi diagram.

Such diagram should be infinite number of diagrams, because infinite number I will have to plot to the represent this e versus k, that obviously is not reasonable. So, what the method by which I can represent the e k diagram is really what we are proceeding towards. So, what we are going to do is we will use the idea of the fact, that underline potential is periodic meaning there by V is equal to r plus R and therefore, use this to represent these energies in a ingenious way, in a interesting way, that would be a first step which I will do in next, today and next couple of next one more lecture.

Following that only after that what I am going to do is, then I going to approximately sure approximate solution for a approximately assume what value V is, right now we are not interested in what the what V itself is. Such that in today's lecture we are going to use the fact that it is periodic that is all, but in subsequently we will introduce we use a approximate value of what v r is. How about the behavior of v r is. Use that to find a analytical solution, using that I will show you that because of presence of v r and its value and its nature, how a band gap can emerge and therefore material can become a semi conductor or insulator.

Having done that to understand conceptually, then of course, then we will we will assume that there is a some residual potential, which we will not we will not really do in this class. But there are real potential based on that people have done the calculations of the band diagrams in the first step you would have learn how to represent e versus k using this relationship right here which is given here. Once you learn the representation and second part we will assume a potential and I will show you the consequence of the potential.

But then the real thing I will show in then e k diagrams, what the e k diagram would look like if the potential is real, but that final one calculation will not be a part of the course because that itself that a course by itself and that is how do u need overview of next 3, 4 lectures how we are going to proceed. So, at this point of time let us assume these two thing that energy relationship is just this. So, you need to represent this energy relationship. Second e versus k diagram, second thing is that my potential is periodic that is what only result we are going to use right now and see what the consequence of this is, all right? So, you may wonder then why did you do reciprocal lattice, very soon you will see that, just today you will see why did we do reciprocal lattice.

They are special vectors and they will do something for us and that is what we are going to do. One more thing we can write down here is solution for this is of form e to power j k dot r that is plain reaction involved. So, using this background let us start this lecture and we will start with what is called as Bloch’s electrons. So, let us start with this what is called as Bloch’s electron.

What is this Bloch’s electron? One that follows one electron Schrodinger equation in a periodic potential, hopefully you see a difference. In free electron that was a only difference, in free electron this potential was 0, otherwise that was also a 1 electron problem. So, here also I am still dealing with a 1 electron problem and I have already shown you the ingenious ways by which a real problem is reduce to 1 electron problem, 1 electron problem. Where the interactions of the potential the potential really represented represented by interactions of all valence electrons, electron pron interaction and also a electron and ion interactions.

So, all those are barred in one effective potential, so that part can be done. So, we have one electron problem in a periodic potential of form V r and has its periodicity of the direct lattice. Lattice periodicity is shown by R remember, what is R? R of course, is my primitive lattice vector defined by n 1 n i a i summation where i of course is 1, 2 and 3. So, in other words I expanded from R is n 1 a 1 plus n 2 a 2 plus n 3 a 3 and this is a vector where n 1 n 2 and n 3 are all integers, in this what happens?

So, Bloch's theorem says that solution to such a problem solution to such a problem remember free electron solution was this, this was free electron solution. Now, question is if you solve one electron problem Schrodinger equation in a periodic potential, whatever that potential is we do not know the potential is, just that it is periodic a help periodicity of direct lattice.

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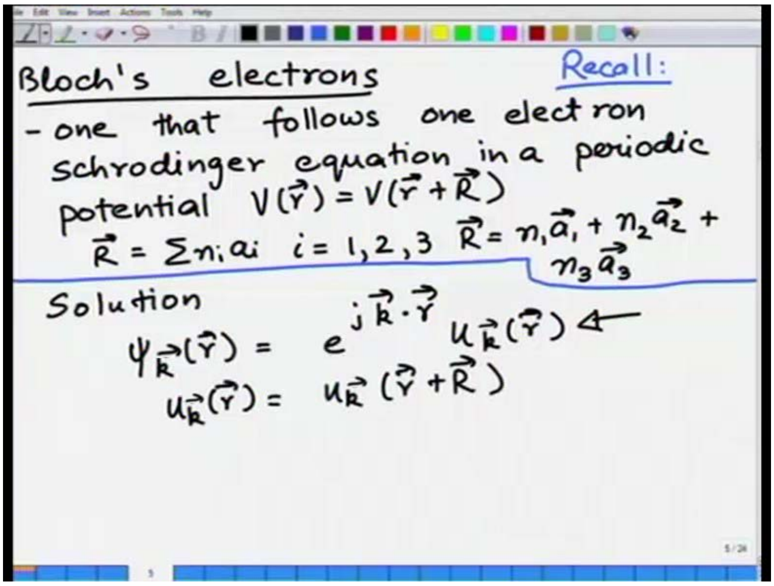

Then if that is the case then the solution is solution of this equation is of form that is of form of e to power j k dot r which we already knew in free electron, but also in a digital term u k r. What is this u k, this u k all we know about this u k is that it is also periodic. So, Bloch's theorem says that whatever the solution, exact solution they are interested in at this point of time, but that if the potential of a periodic then solution will be of this form where u k will be periodic that is a Bloch's theorem. So, that is a solution we are going to use and see which of solution will be of this form, the fact that solution of this form itself gives us a huge amount of information and that is what about this lecture will be about this part only, so let us look at that.

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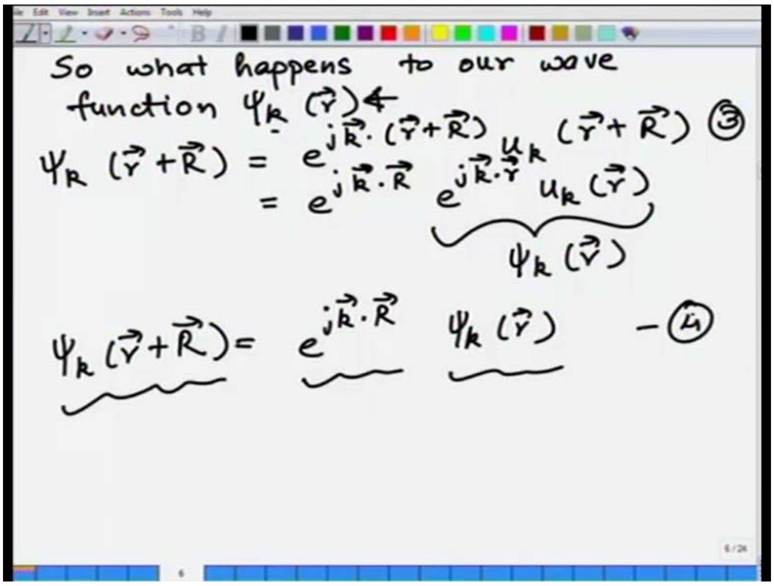

So, what happens to wave function and notice I am using a subscript k, because this corresponds to some value of k, k can be there are many many k values will any k value will satisfied this Schrodinger equation, real solution will therefore summation of all those k values. Hence, I am putting a index k for a for a k value. So, with that let us write this solution, what will happen to phi k at r plus R that is the question we are asking. Wave function at k this we have derived in the previous equation, I have written it here by it here, this is what we have written here.

Now, what we are doing is we are asking what will this quantity will be equal to? This quantity let us just substitute in therefore, so that we are going to write as e to power j k dot now r plus R and u of k which will be r plus R. So, that is what this quantity will be is equal to I just substitute in there. So, now, what happens? What is that mean? That mean maybe we should keep labeling the equations also, let us call this as equation as number one, let us this as equation as number 2, let us this as equation as number 3.

So, now look at equation number 2, equation number 2 says, so let us write this first down first. So, this quantity will be equal to e to power e to power j small k capital R times, what e to power j small k dot small r. Now, I am going to use equation number 2 which says, let us use equation number 2 which says u of k r plus R is same thing as u of k at r that is periodic, so I am going to use that. So, I am going to replace this by u k just r. Now, what is this quantity equal to? By equation one this quantity equal to simply phi of r, that is quantity simply phi of r.

So, therefore phi of k r plus R is equal to e to power j k dot r phi of k at r and all these are vectors and that is just this quantity, what is that mean? Wave function in one primitive cell differs from another primitive cell by a quantity by this, by a quantity by this, its differs by. So, this a phase difference in wave equation between, lets limit this equation between one cell and another cell, there is a phase difference in the wave function that is what we have figured out.

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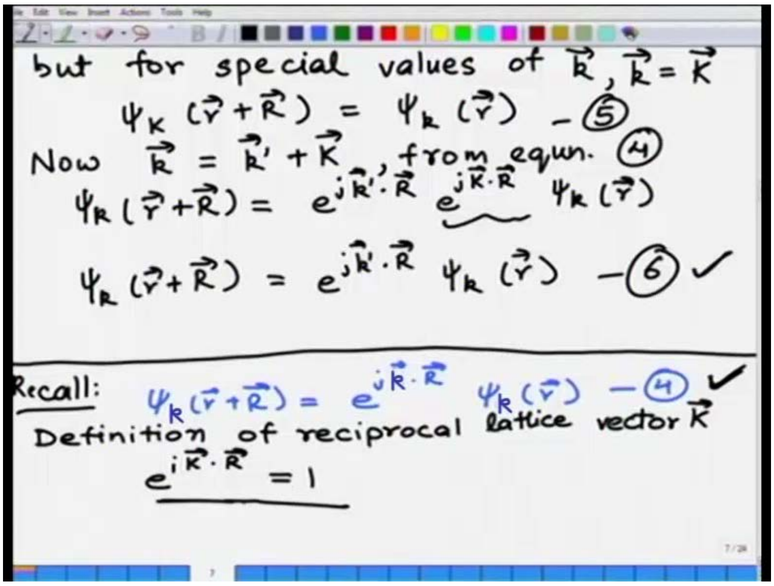

But for a special values values of k meaning for k equal to capital K, remember now here comes the reciprocal lattice vector, this is a special K is remember that is reciprocal lattice vector. Now, for this values what will happen? If you substitute capital K for it, then phi of capital K r plus r will become equal too, if you substitute capital K in there, in this in this equation number four if you substitute capital K. Then do you remember the definition of the reciprocal lattice itself was that e to power j capital K dot capital R was always 1, that is how it was chosen.

Now, you can see why chose we that that way, in that case phi of capital K would be equal that is equal to 1, therefore this will happen. Certain lattice points reciprocal lattice points when small k or sorry not like this point, a small k was becomes capital K for those vectors, in that case vectors which are pointing towards lattice cell versus another cell would be identical, all right? So, that is important result. Now, let us once proceed further, now let us do a trick, if that is capital K is special vector, then if I have a small vector k let me do this, let me do little trick and express this as another any small vector k k prime another another plus capital K vector I can always split any vector in to sum of two vectors.

But just that I want to make sure that one of those vectors is capital k, so if I take the small k to be like this, then what happens? Let us look at this. So, from four then from equation four what happens? Just look at this phi of k r plus r will become equal to just lets substitute in their, so that will become equal to e to power j k prime dot r in to power j capital K dot R. Since, this quantity is equal to 1, therefore phi of k r plus R, this will be equal to j k prime vector R phi of k r and let us call this equation five.

Now, let us call this equation six lets call this equation six. Now, can you compare equation number four and equation number six, compare equation number four with equation number six, what do you see? Something interesting isn't it? Notice that they look the same if you place k by k prime, if you replace k by k prime it makes no difference, it makes no difference is means the same.

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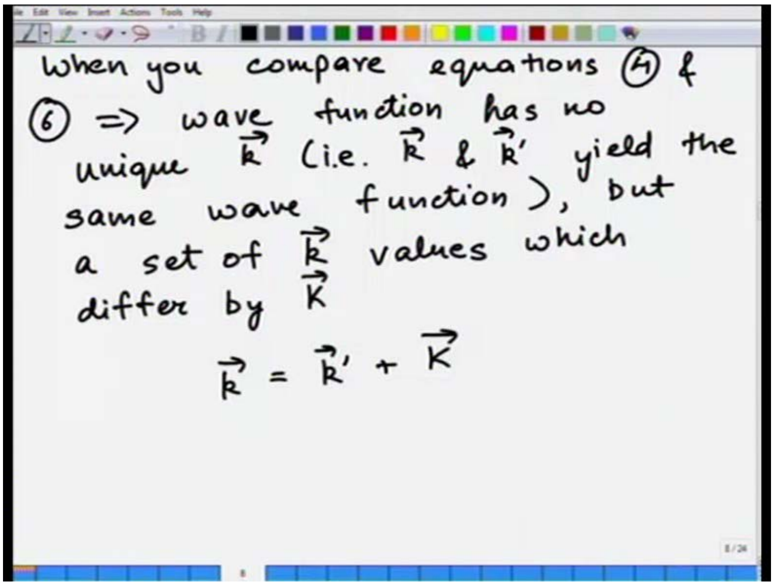

So, when you compare equations four and six, if compare equation four and six implies wave function has no unique k, that is k and k prime yield the same wave function, unique k, but a set of k values which which differ by capital K vector. Now, you can see why is that reciprocal lattice vector, reciprocal lattice vector is special. Remember k was equal to k prime plus K, so these two vector differ by k prime.

And k vectors differed from each other by some k vectors by a capital k vector, as long that is true then the wave nature of wave function remains the same. Wave function does not change; that means or that gives us a handle, that gives us a handle. So, now this this conclusion which comes out of a Bloch's electrons from the fact that single electron periodic potential we can now begin to use them for our purposes.

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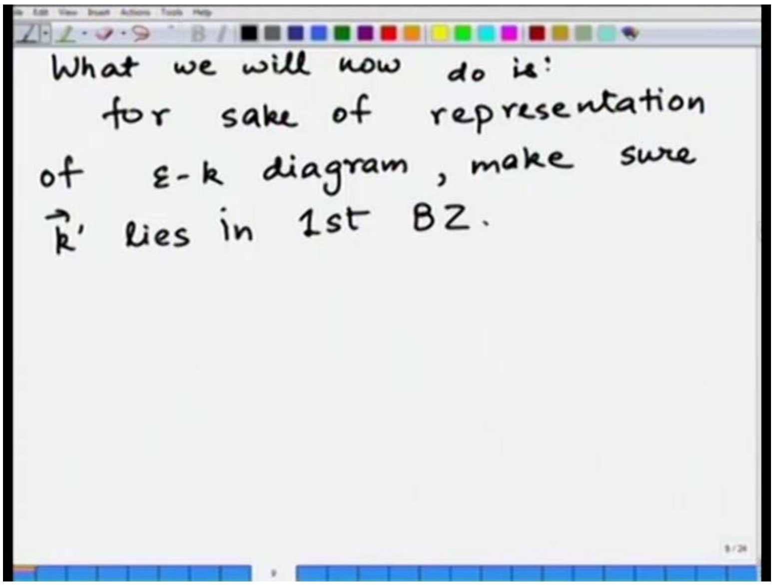

So, what I am going to do is show you what it means how does one reduce this problem. What I am now going to do is, will now do is for sake of representation of e k diagram, make sure that k prime lies in first. Do you follow that? Why I want to do is, since it does not matter k you can choose as long as if I have a small k vector. I can always find a small k I can find a small k prime vector which and the these two vectors different are different by a capital k vector and it does not matter, if I find a small k vector wave function will remain the same.

So, that is the logic I will use and I will make sure that the vector I find that is k prime vector always lies in the first and then instead of plotting e versus k diagram, I will plot e versus k prime diagram. Now, since k prime is always in first (( )), therefore the k axis does not need to go to infinity instead it is only confined up to the boundary of the first (( )). You see that is the first thing we want to do to limit our size of the band diagram. So, in order to do that let me show you a little bit how we can do that.

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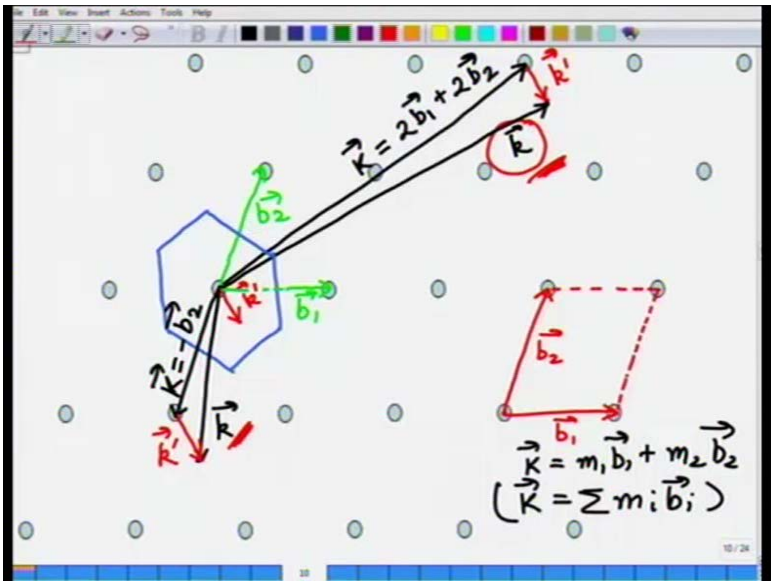

So, let us take this is as example, this is the same example which I had shown you for a reciprocal lattice where I showing you brag refraction condition, construction of belanzone. I had shown you construction of belanzone in a two dimension and three dimension the same construction which you do. So, I am showing you again going back to the same same diagram which I have drawn in the previous lecture in that direction were my b 1 and b 2 were my lattice vectors and therefore this k was equal to m 1 times b 1 plus m 2 times b 2 in general of course, k is equal to m i b i where m is the summation where m summation is over i is equal to 1 2 3 write 1 2 3 in genral.

But Since this is a two dimension problem instead I am going to represent here, so k is of that and this is lattice which I had shown you. Blue line I had shown construction I had shown you that was a belanzone. So, now, what I am going to do is I want to show you is that choose whatever k you want choose whatever k you want will always represent, will find a k prime which lies in the first belazone, let us do that, let us take there is an example. In order to do that lets do it like this, that let me remain consistent with this example I have chosen, so that the construction is easier.

So, let us go somewhere here, let us go somewhere for example, let us go somewhere here. Suppose, this is my k vector, suppose I choose a k vector which looks like this, suppose I have k vector which is like this, this is my k vector, this is my k vector. If this is the k vector I can always find a capital K vector which is reduce my k vector in to the first belanzone, let me show you that is the example.

So, what we do is we choose another capital K vector which is like this, remember capital K vectors are those vectors which are drawn by or I will write it more explicitly here. So, this capital K vector then is equal to lets choose the value of m 1 and m 2. So, this is 1 and 2, so 2 b 1 2 b 1 plus this is 2 b 2 this is the capital K vector I have chosen, if so then what is k prime vector? This is k prime vector. So, this is k prime vector, it is k prime vector it is k prime vector I can represent the same k prime vector by here. Draw the same parallel vector from this origin because origin must remain the same because the k prime vector.

Now, notice I will show you that it does not matter it does not matter this k prime is not unique vector, many such k vectors lead to same k prime vectors that is what I want to show you from this diagram, it does not matter. This is second conclusion I want to show you, first I have shown you that if you give me this k vector, if you give me this k vector I will find you it is always possible by taking a neighborhood lattice point. That means, capital K vector it is always possible to reduce to another k prime this is within the first belanzone, you can see this is within the belanzone.

Second statement I am making here is that this k prime is not unique, this k prime is result of many different k's it is possible that is from very small k's. This k prime could be same and that is example I will show you now. So, for example, let us take it like this, suppose you want to take somewhere here like this, suppose this is your k vector, another k vector which is like this, this is your small k vector. So, in order to bring this into first belanzone, let me choose this as my capital K vector, this is my capital k vector this capital k vector you can see now is my minus b 2 vector, it is just a minus b 2 vector, remember this is b 1 and this is b 2, this is b 2 and this is b 1, it is just minus b vector. So, therefore what does it mean?

This means that this is k prime vector, if that is the case then you see this k prime vector is same as this red colored k prime vector I have shown if I transfer to (( )). So, whether it is this k or whether it is this k, both leads to same k prime. So, now what are the conclusion we draw, next page I am going to write down write down the conclusion which which I draw from this. So, what, but let me say in it words now one more and I will repeat it again. So, as a consequence of a periodic potential Bloch’s therom said that, first I should told you that is always possible, not always possible.

It is possible to reduce the problem to 1 electron problem with an effective potential, number 1, number 2, once I have one electron problem, then a 1 electron problem is being solved by in periodic potential which is natural to assume, since the lattice has a periodicity so the potential should also have the same periodicity of r. If there is a periodic potential, then there is Bloch’s therom which gives you formal solution, given that form of Bloch’s that form of a solution.

What we are able to tell is that wave function in one premitive cell to another premitive cell is different by a only a phase. But for a special values of k there is no phase difference that is number 1, number 2 conclusion we maid was that wave function, there are many many different values of small k is which is lead to a same wave function which is lead to a same wave function, we have use this as a consequence of Bloch’s theorem. We will use this result to show that if you have. Remember I saw it seeing at when I want to plot e k diagram, I have infinite values of k possible and you extend of course, how far it can go with a infinite extend.

Now, since any k value which you have I can always represent by a small k, I can represent by a k prime vector which has within in the first at least what we have achieved is that we have confined that infinite extent of this k vector within a narrow fun fine of a first only. That means, that much we are able to do. So, let me write down and second thing I have shown you is there is no uniqueness, whatever k prime vector you find the same prime k vector represents many different many manymanymany infinite number of not infinite very large number of small k vectors.

I have shown you two examples I have taken this k vector and I have taken this k vector and I have shown to you that by using an appropriate capital K vector, reciprocal lattice vector you can reduce it that to a small k prime vector which are both are same. Both are within the first belanzone that is a red line which I have shown you, so that is a reciprocal lattice vector. So, let me write down the conclusion here.

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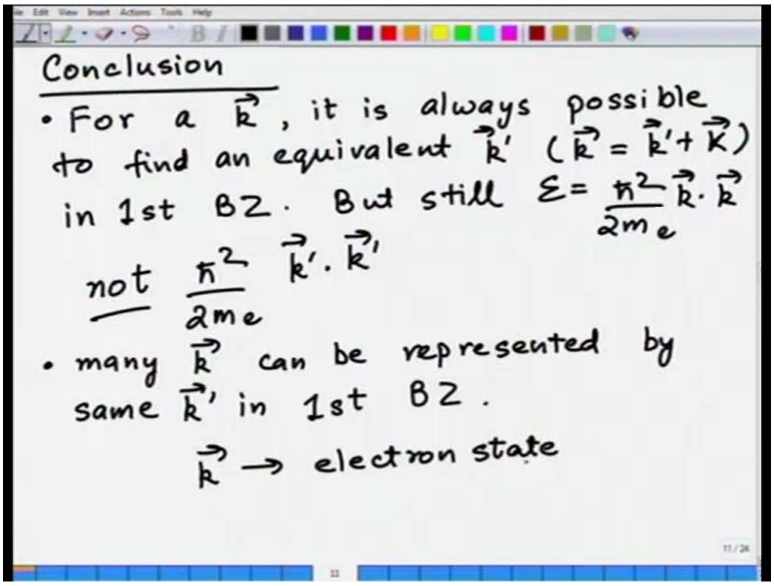

So, conclusion number 1 for a k value it is always always possible to find an equivalent k prime which differs from k by amount capital K only. It is always possible to find an equivalent k prime in first belanzone, that is point number 1 I have conclusion, but still but still energy is equal to h square by 2 m k dot k knot h square by 2 m e k prime dot k prime, it is not that. Energy is still, so x axis of e k diagram I can find k prime, but the energy that I represent it is still going to be real energy which will use be using k not k prime. So, that is the one point that is one point I want to make. Second within this conclusion set one is that many k values can be represented by same k prime in first, that is the conclusion I want to draw.

So, if these are the two conclusion m then now you can see. Now, therefore since it is same k prime in first belanzone I can, this k vector small k vector represents, k vector represents electron state. Remember in free electron theory we found that this is discreet and some state which electron can take, this k vector represents electron state and this can represents and many many this k states k can be represented by same k prime within the belanzone. So, question I want to ask is that in one therefore, how many natural question to ask is how many electrons can I put? How many k states therefore, are available only within the first belanzone itself, in first belanzone how many case states are available?

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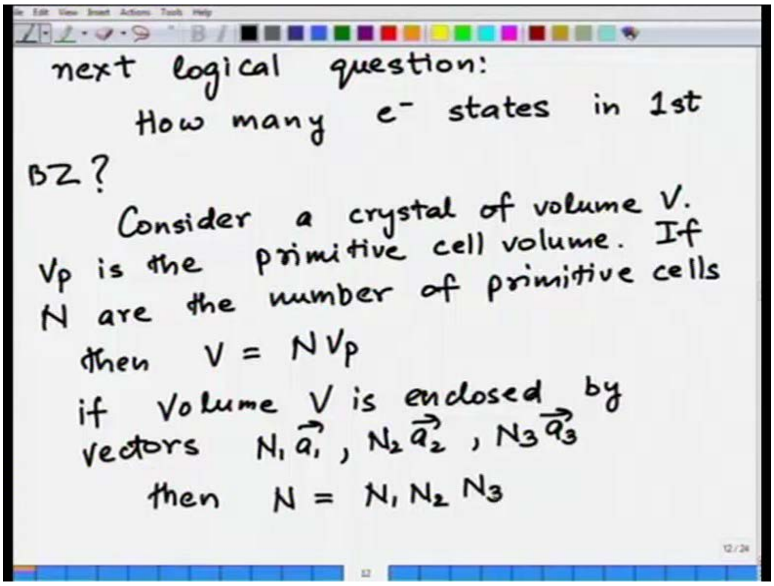

So, that is when next logical question is next logical question is, because k prime k prime represents many k states a small k states therefore, and this k prime is in first belanzone. How many total amount of states are there in the first belanzone? That is the question we are trying to ask and since once you known a number of states, then we known how many electron we can put in the first belanzone. Next logical question is how many e states in first belanzone, that is the question we are have to answer now. In order to do that let me do this, consider and I just do a simple algebraic calculation.

Consider a crystal of volume V and you see a primitive cell has a volume V p is a primitive cell volume, if n are the number off primitive cells, then clearly V is equal to N times V p. Now, assume that remember, so if volume V is enclosed by vectors N 1 a 1, N 2 a 2 and N 3 a 3, so think of this like this, that if in N 1 times in direction of a 1, if N 2 times in direction of a 2, N 3 times in direction of a 3, that is the extent of my total volume. That means, so I take a in terms of primitive lattice vectors, if I take N 1 steps in a relation of a 1, N 2 steps in direction of a 2, N 3 steps in direction of a 3, then I construct my whole volume.

If that is so, then clearly N is equal to N 1 multiplied by N 2 times N 3, so how many primitive cells there are therefore, if I took N 1 step in this direction, N 2 step in this direction and N 3 step in this direction. Then total number of primitive cells which are defined by 1 a 1 a 2 a 3 will be N 1 into N 2 into N 3, then that many primitive cell. I have said N is that number of primitive, total number of primitive cell in volume V. Therefore, this N must be equal to N 1 N 2 and N 3, to the whole extent of the volume is determined by the multiples of a 1 a 2 a 3 which I have N 1 N 2 and N 3.

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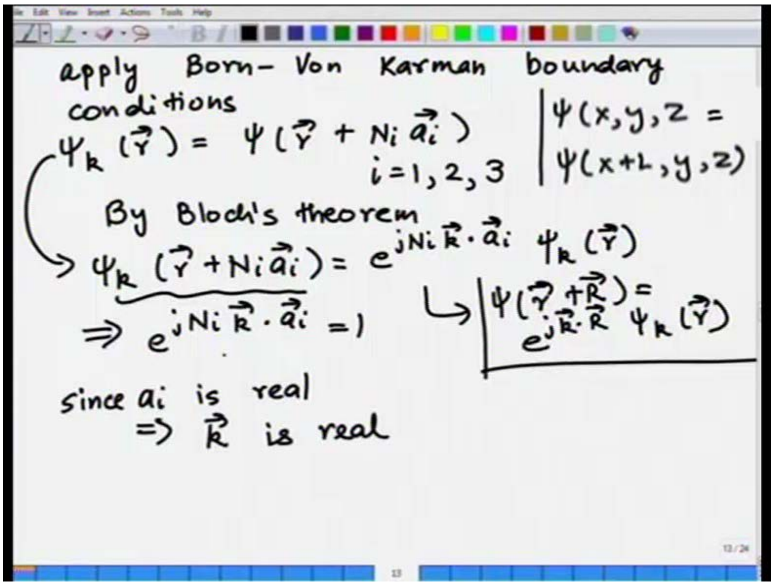

Now, remember we apply again there are good old Born Von Karman boundary condition, we apply which was what you will recall in free electron theory. I have written phi of x comma y comma z being equal to phi of x plus l y comma z you will recall, I have written it something like this. In as a Born Von Karman boundary condition namely there what goes in it is like this, if something comes out of here, it basically entered from that side, it has entered from the other side of the boundary, if this boundary then it is comes out something comes out here, essentially enters from this side.

As a poster saying let us make the wave function 0 on the both sides, so it does not leak. In order to avoid the leak of wave function, confined the wave function of material itself, what we are used was Born Von Karman boundary condition, a cyclic boundary condition we said we will not allow the wave function to leak out of the material, but the way we will do it is that whatever coming out of here it goes back in from the other side. So, that is now we are going to write the same, so now the material boundary is defined by the multiples of N 1 N 2 N 3, so we will use it in that context.

So, I am going to write therefore in that case, phi of k at any position r will therefore be equal to phi of any position r plus N 1 N i a i were i could be equal to 1 2 or 3 not summation 1 2 or 3 it is just like this. If you where is boundary in this direction after N 1 this is the a 1 direction, so after N 1 times I have my boundary here, that is why I have written N 1 multiplied by a 1 or if it is in direction a 2 it is N 2 times a 2 is in count of my boundary. So, I have written it like that in general form where i is the square quantity.

So, now by Bloch's theorem what happens? By Bloch's theorem phi of k of r plus this N i a i this is vector, a i whatever N i is you know as 1 2 or 3 and you apply in equation in 1 2 there, this at period is equal to e to power j times, now I am going to write this is n i k dot a i, I am going to write like this now phi of k at r. Remember where this come from? This whole stuff comes from phi of r plus R being equal to e to power j k dot r times phi of r, that was Bloch's theorem solution, that is what I have applied here essentially. What is that mean? It implies if you substitute in there.

So, what is that mean? Since, this quantity should be equal to remember use this equation here, since this quantity should be equal to phi of r implies that e to power j N i k dot a i should be equal to 1, that is what it implies. So, if since a i is is real, it is direct lattice vector it is lattice vector, so it is a real quantity and if it is real quantity then dot product. So, that means k must also be real otherwise I would have got in an imaginary implies that k must also be real. If k was not real then I would have got in an imaginary component also, so therefore this implies that k is also real.

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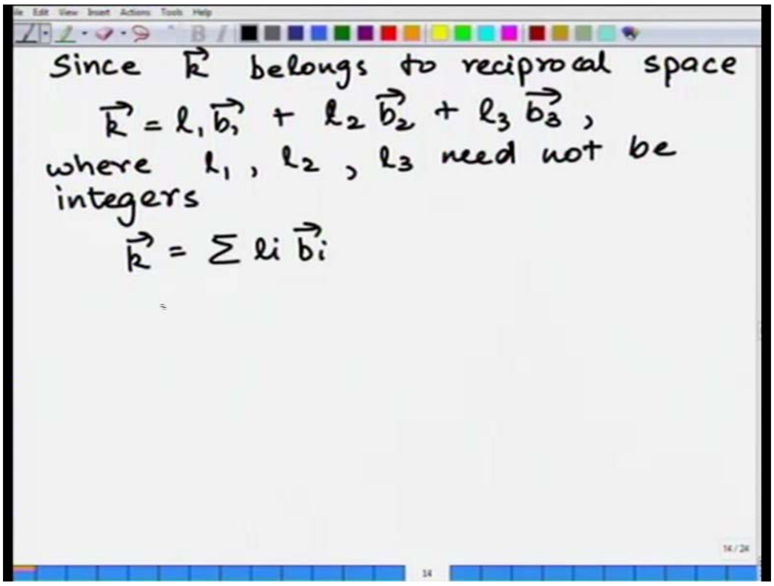

So, what I am going to do is therefore, since k belongs to reciprocal lattice since k not to reciprocal lattice, k belongs to belongs to reciprocal space, I am just going to express this k vector also as some multiples of l 1 times b 1 plus l 2 times b 2 plus l 3 times b 3. And these are reciprocal lattice vectors where l 1 l 2 l 3 need not be integers because if they were integers then then the small k will look like capital K vector. So, it is just I am trying to do is let us express we have b 1 b 2 b 3. So, let us express k as some multiple some coefficient of that l 1 l 2 and l 3 we are going to choose and use that. Which I am going to suficly write as summation over l i and bi, so that you get the idea that i is 1 2 and 3. So, now as I said these all are not necessarily integer.

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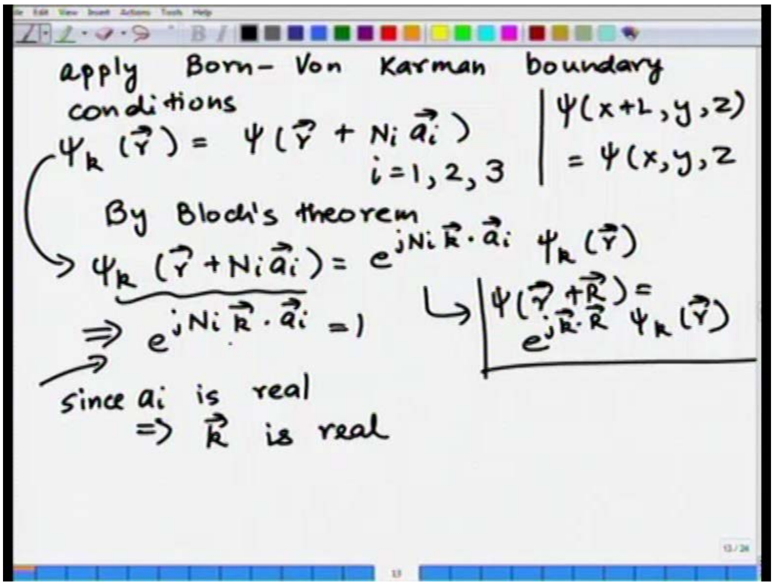

Now, since we have since we have that exponential, so now let us substitute this k, since we let us go back to our equation here let us go back to this equation here substitute in here it called j N i k dot a i, so we will use this e to power e to power j let us j N i k dot a i, let us substitute in there, so what we get here?

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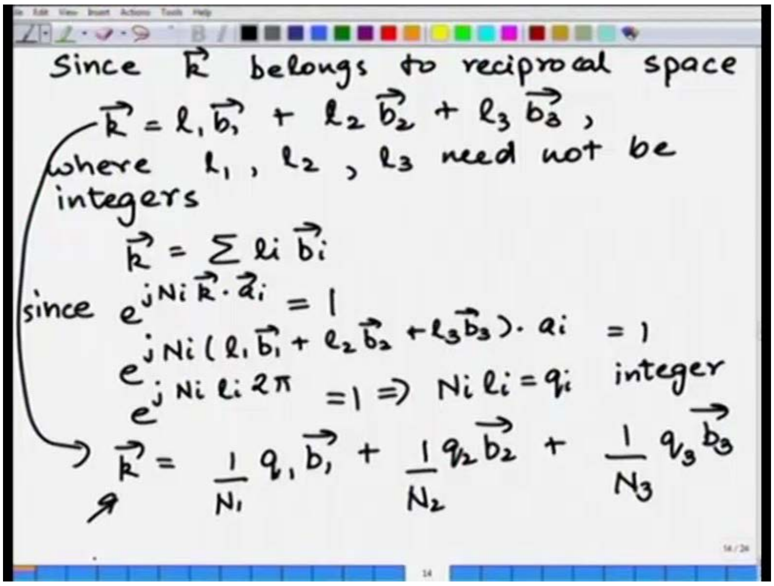

So, what we get is e to power j N i for k we substitute l 1 b 1 plus l 2 b 2 plus l 3 b 3 b 3 dot a i equal to 1, what is that mean? Remember whatever i value is i 1 2 3 then you will pick only that l 1 or l 2 or l 3 according to that in the dot product. So, therefore e to power j N i l i is what we get picked out of this and b i dot a i will it to 2 pi, so I should put a 2 pi that should be equal to 1, that dot product of a i and b i is simply 2 pi. You can see our definition of b i, the reciprocal lattice vectors, this implies that N i into l i should be an integer, this quantity should be an integer and let us give it a name let us give it a name of let us say just call it q i, just give it a name of q i, these is a integer.

So, this quantity should be integer quantity what is that mean? That means k vector should be equal to i by N 1. I am going to substitute in here and here from here I am going to write k as l 1 which to 1 times b 1 divided by 1 by N 1 plus a integer quantity q 2 times b 2 divided by 1 by N 2 plus 1 by N 3 q 3 times b 3. Now, what is the volume enclosed by this case state what is the volume as a consequence of this state.

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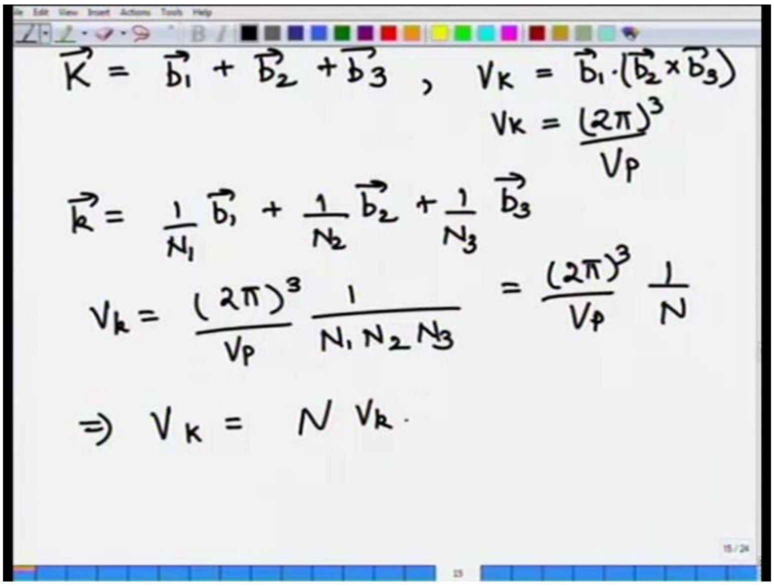

Remember a vector k which is due to b 1 plus b 2 plus b 3 primitive cell leads to a primitive cell volume. This primitive cell volume is will be equal to this b 1 dot b 2 cross b 3 will be just this quantity, that is the volume of the primitive cell in the reciprocal space. Similarly, if you look at this k, what will be the volume occupied by this case state and this quantity is of course will be equal to you can see 2 pi whole cube divided by V p that you can carry out this as a exercise. Likewise and reciprocal space imagine equalent to that you think like this, these are integer, these are integers quantities, these are integer quantities.

So, similarly I am going to write what is the volume volume occupied by this k state which is defined by 1 by N 1 b 1 plus 1 by N 2 b 2 plus 1 by N 3 b 3. What is the volume occupied by this? This is a one case state occupies this small k volume which will now in this case will simply be, if I substitute in their then instead of b 1 I will substitute b 1 by N 1 instead of b 2 I will substitute b 2 by N 2 and therefore, and b 3 b three by N 3 I will substitute.

If I do that substitution then I will get this as 2 pi whole cube divided by V p divided by 1 by N 1 N 2 N 3 which is equal to 2 pi whole cube V p times by by N. That implies that volume of primitive cell should be equal to volume associated N times what the volume associated with a case state and what is the implication of this? Implication of this I will write in next page and finish the lecture here.

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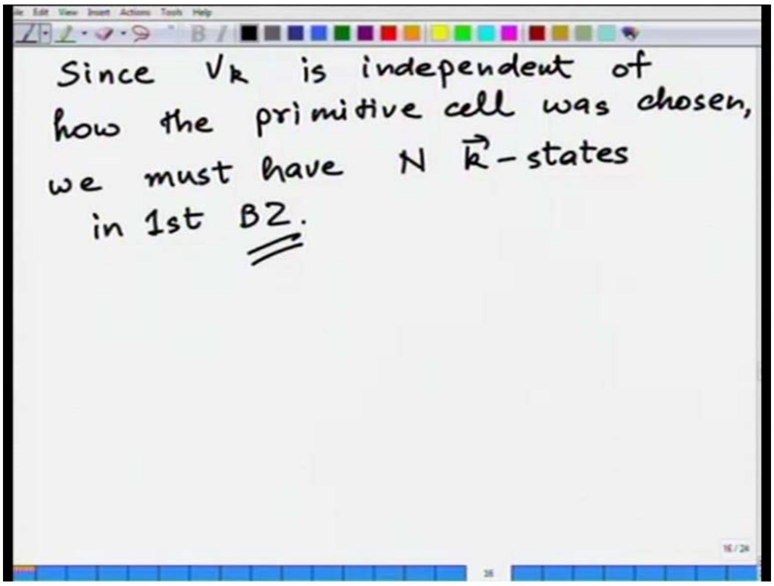

That since V k is independent of how the primitive cell was chosen, so this result must be true as a general case. So, that means I should have; that means we should this equation therefore says, since this is a volume associated with one case state, in first belanzone and this the total, this is the volume of the primitive cell. Since that means, I should have and belanzone represents that means, a primitive cell in the volume of the belanzone that means, primitive cell in reciprocal space is really a belanzone.

So, therefore this is the volume belanzone, so this is a volume belanzone associated with one case state; that means I should have N case states in the first belanzone. We must have N k states I wish again put N first belanzone, this is about to end my lecture and shown you now that means, if you had N primitive cells in the real lattice, in the real material which has given to you, if you have N primitive cell, then you have N k states available in the first belanzone. So, you know how many electrons you can put in that, how many first belanzone will contain how many electrons.

So, this is the conclusion in we have drawn, we will use these two facts to now draw out our e k diagram. So, from in next lecture on what I am going to do is, I am going to fist show you how e k diagram could be drawn for a hypothetical one dimensional system. Then what I will do is then I will take it from metals and I will show you how e k diagram is to be drawn for three dimensional system, for say aluminum or copper or some material like that and in from that point you will start appreciating what e k diagram is. After that we will introduce a actual potential and see how the band gap origin originates.

Thank you.