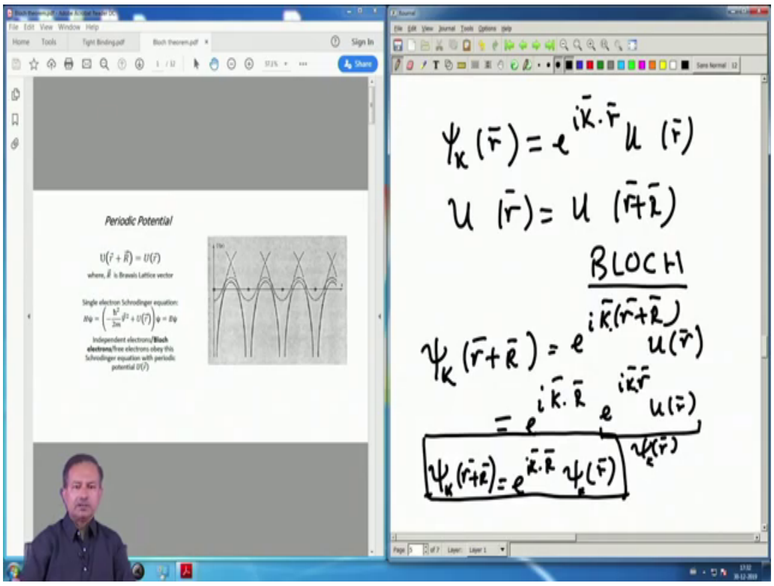
Electronic Theory of Solids

Prof. Arghya Taraphder
Department of Physics
Indian Institute of Technology, Kharagpur

Lecture – 14
Proof of Bloch's Theorem

Hello again. So, we have been discussing the periodic potential and how an electron behaves in a periodic potential.

(Refer Slide Time: 00:29)



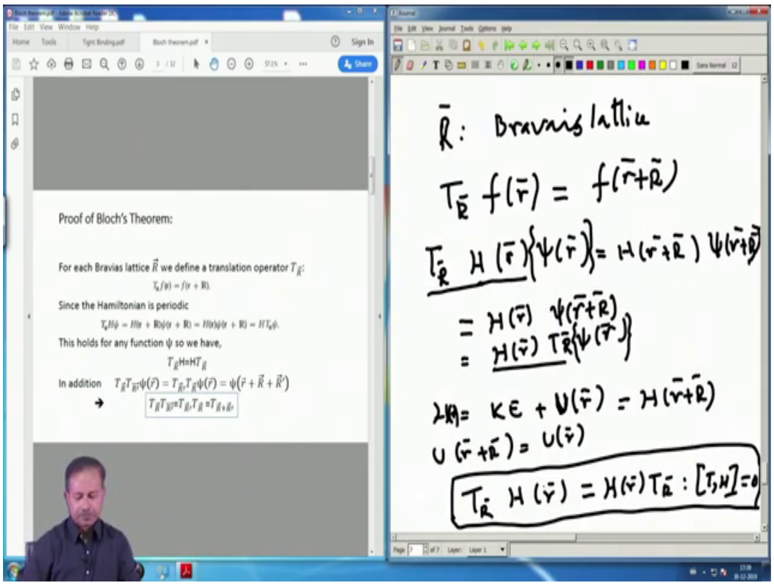
So, our intention again is to solve for the Schrodinger equation, solve Schrodinger equation in a periodic potential. Now, periodic potential as I said is a potential which has a periodic repetition. As this one-dimensional figure shows that this is, so this picture basically shows that U r plus R is U of r. Here in one-dimension of course, R is just a one-dimensional quantity whereas, in a two and three-dimension higher dimensions these R has to belong to that Bravais lattice that I have showed in the previous view graph previous class.

So, the idea is that the if you have to solve this the under this condition that the potential is periodic then the Bloch had come up with the beautiful theorem which did not give us the solution exactly, but it told us about the solution. It is very very powerful theorem. It told us that the solution must be such that it has a periodicity of the lattice, in the sense that it is a plane wave multiplied by a function which bears the periodicity of the lattice. So, that function U of r is a periodic function exactly the same period as the potential and it is multiplied by a phase factor e to the power i K dot r.

So, it is a plane wave multiplied by a factor U which is a periodic with the same period as the potential. So, that immediately implied that the wave function if you translate by a Bravais lattice vector the wave function is just pick up a phase, nothing more and that phase is e to the power i K dot r. What that K is? Requires to be solved and so that is the details of the solution, but at the moment just see the beauty of this solution.

The solution tells us that at any point if you find out the psi of K of r in the lattice you know the solution at any other point in the Bravais lattice, on any other lattice an any other point separated by a Bravais lattice vector. So, that is a beautiful theorem because it is just the lattice has all these points, lattice points and if you find a solution in one point you should know the solution at any other point of this lattice, ok.

(Refer Slide Time: 03:29)



So, let us see how it turns out. So, this is what I have already informed you. Now, I will not go to the details of the proofs, but there is a beautiful way to look at the Bloch's theorem and it is a proof which uses the symmetry of this of translation operator.

So, let us just a get to it; this thing basically shows you there are the Bloch's theorem has to be correct and the these reproduces Bloch theorem. It does not disprove, it does not tell you that what that wave function is or nothing about it. I mean something about it, which is basically what is Bloch theorem. And it comes from the fact that the wave function has to be an eigen function of the translation operator as well. So, let us see what this proof of Bloch's theorem is.

You can find this proof in many places. For example, in Ashcroft and Mermin's book, but in many other places you will find this argument; so, very simple argument. So, let us just go through this argument. So, take each Bravais lattice R. So, take any Bravais lattice R and define a translation operated T of R. So, if R is a Bravais lattice point, R belongs to the Bravais lattice then T of R is an operator, operates on a function f of r to give me f of r plus R that is the definition of T of R, ok.

So, the T of R function, T of R operator operates on a function f of r and gives me the function at a point which is r plus the Bravais lattice R, in Bravais lattice vector capital R. So, this is what T of R does. So, this is called the translation operator. Basically, T of R translates the wave function the function f of r two a distance capital R, that is all, vector addition of r, a small r with capital R. Now, let us look at this property its property.

Now, we know that the Hamiltonian is a function of R of course. So, let us operate T of R on this H of r psi of r. So, it gives me H of r plus capital R psi of r plus capital R, right that is the definition of T of R. Now, this is since the Hamiltonian is periodic with respect to R. You remember that Hamiltonian is basically kinetic energy which is a del square operator plus these V of r and V of r or U of r and U of r plus R is equal to U of r and kinetic energy being a del square operator it does, it does not care by a rigid shift nothing happens.

So, this is basically the same; so that means, that H at r is same as H of r plus R because U of r plus R is equal to U of r. So, if that is true then I can just write this again as H of r psi of r plus R. Now, psi of r plus R is basically nothing more nothing other than T of R psi of R, right. So, what has what has happened? That means, I operated with T of R on this function T of R into H of T of R times H of r, these are my operators.

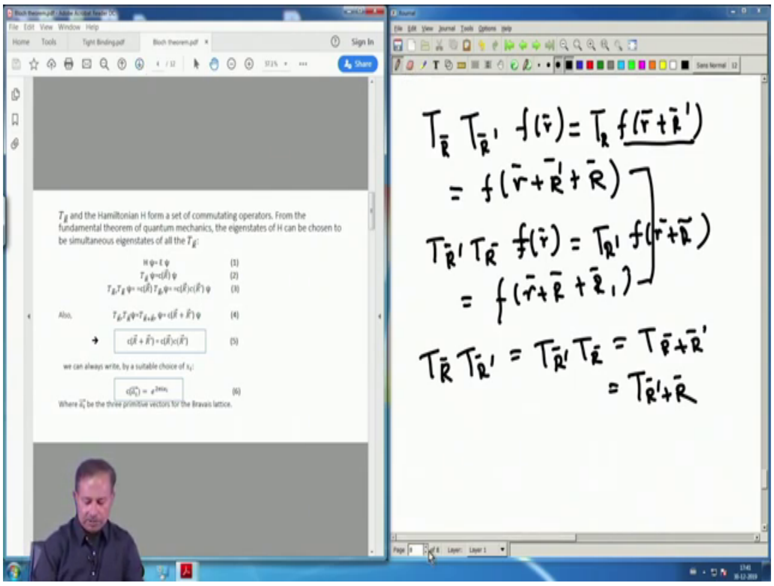
It operated on this wave function psi of R and what I have is H of r is T of R operating on psi of on psi of r is the same as that; that means, T R operator into H r operator is the same as H r operator into T R operator, that means, this two operators commute T R H equal to; that means, T and H commute. So, that's obvious, right.

I mean this is this tells me that T and R, T of R and H of r, H the Hamiltonian just commutes, ok. So, these two commute means something very important in quantum mechanics. In a in quantum mechanics if two operators commute, then of course, you can choose their simultaneous wave function. You can choose the wave function which is simultaneous wave function of both of them.

This is very simple to prove. You can just take it as an exercise and a check it for yourself. If you cannot then there are 100s of places where you can check it, even in the internet you will find the proof of that that is just a few line 2-3 lines that you have to work to get this done to get that result, ok. So, that means, I can choose simultaneous eigen functions of both H and T of R these two, these two operators. Again remember that we have not yet gotten the solution.

I mean this is solution is still not obtained, but we are obtaining properties of the solution. So, this is one property that we immediately got from this argument is that the operator the eigen function will be such that it can be chosen I can choose the wave function in such a way that it is a simultaneous eigen function of both T of capital R and H the Hamiltonian. So, that is one thing that I just learned, ok.

(Refer Slide Time: 10:27)

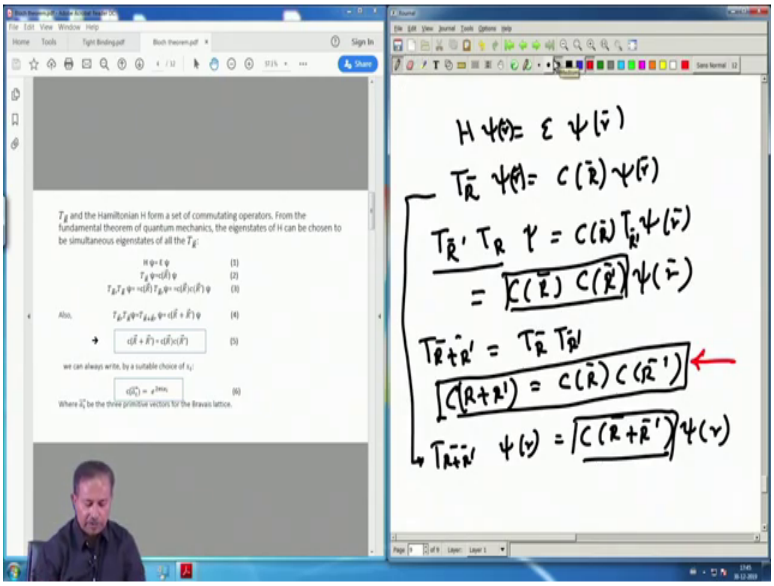


Now, let us just look at what T of R, the property of T of R. So, they take two Bravais that is vectors T of R and T of R prime. Now, operating on a function f of r for example, so, will give me T of R f of r plus R prime, right. So, that is equal to f of r plus R prime plus sorry R prime plus capital R, right. This is obvious because I first operated with T of R prime I get f of r plus R prime. Now, I operated with T of R on this function on this whole function whole thing then I get f of r plus R prime plus R, ok.

So, now, let us look at the other way T of R prime, T of R. So, that gives me f of r of course, that gives me T of R prime, f of r plus R equal to f of r plus R plus R prime which is the same as this one. So, these two are the same. So, that means, what? That means, T of R, T of R prime equal to T of R prime T of R equal to T of R plus R prime equal to T of R prime plus R as well. So, this is another corollary of this T the way that T of R operates on a function, ok.

So, let us just see what all these things give us. As I said since T R and Hamiltonian commute I can I can choose a wave function which is a joint wave function of both of them. So, that is the fundamental theorem of quantum mechanics and let me just assume that I can do it I mean, I have just shown that I can do it.

(Refer Slide Time: 12:59)



So, let me just find write down H psi equal to E psi and T of R operating on psi will give me some function of this is a eigenvalue, but it has to be a function of capital R; obviously, and psi of R, ok. So, this is I can choose this, my psi can be such that psi is a simultaneous eigen function of both H and T of R and these are the two eigenvalue equations that I have written down.

So, this theorem that I just use I just proved the relation that corollary relation that I just proved let me use that T R prime R T R of psi is equal to c of R. Now, psi r plus R prime, so these so this is c. So, you remember T of T R of psi is c R of psi. Now, c is just a function and so, T of capital R it is not a function of small r remember, so I can take T of R prime here. So, now, T of R prime of psi of r is c of R prime psi of r, ok.

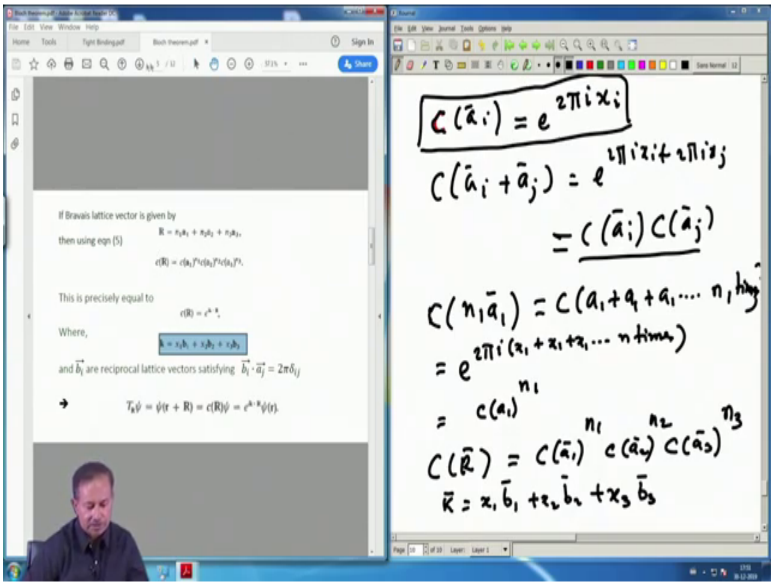
So,; that means, that and then we also know that the T of R plus R prime equal to T of R into T of R prime. So, that means, c of R plus R prime must be then equal to c of R into c of R prime, right. Because you see T of R into T R prime into R is equal to T of R into R prime has to be equal to T of R plus R prime. Now, T of R prime T because T of R plus R prime of psi of r is nothing, but c of R plus R prime psi of R according to this equation, right.

So, that means, this relation has to be correct. The form of c of R plus R prime, so that this equation gives me a c of R plus R prime the I already know that T R into R prime is c of R into c of R prime, so that means, c of R T of R prime. So, this is c of R prime c of R into c of R prime psi of r is the same as c of R plus R prime psi of r. So, that that just basically let us me equate this part with this, ok. And that is what this is. This equation is all I need.

So, now I can choose my c of R. So, for example, let me choose as shown on the left. Let us choose a c of a sub i. So, a are the three primitive vectors that in three-dimensional for example, we chose for the Bravais lattice. So, let us if we are working in one-dimension then life is simpler, I only have to choose one a 1 that is all, but suppose we are in three-dimension then we will we can also do it without any complication we can choose c of a i.

So, this is a perfectly valid choice, that satisfied that equation I just wrote down; c of a of i equal to e to the power twice pi i x of i, ok.

(Refer Slide Time: 17:31)



So, this choice clearly gives me c of a i plus a j equal to e to the power 2 pi i x i, e to the power 2 pi i x j which is e to the power, so this is a c of a i. So, these for example, let me write it this is then plus, and this is c of a i, a i and c of a j, ok. So, it is a perfectly legitimate choice which satisfied that previous relation that I found out c of r plus R prime is equal to c of R into c of R prime. It satisfies that.

So, that means, this choice that I have just made is perfectly legitimate choice. I can choose like my c of a i in that form, ok, ok. So, let us go ahead and see what we do with it. Any

Bravais lattice vector for example, is given by R equal to n times a 1 plus n n 1 times a 1 plus n 2 times a 2 plus n 3 times a 3 as we showed. So, that means, that c of R I can immediately write as.

So, what does it mean? That c of suppose, you need c of n 1 a 1, ok. So, what will you do? You will basically write n, basically n times you will write c of a 1 plus a 2 a 1 plus a 1 plus a 1 n 1 times, right. And then you can use this theorem that e to the power 2 pi i x 1 plus x 1 plus x 1, n times. So, that will give you c of a 1 to the power n 1 that is all by this relation, ok.

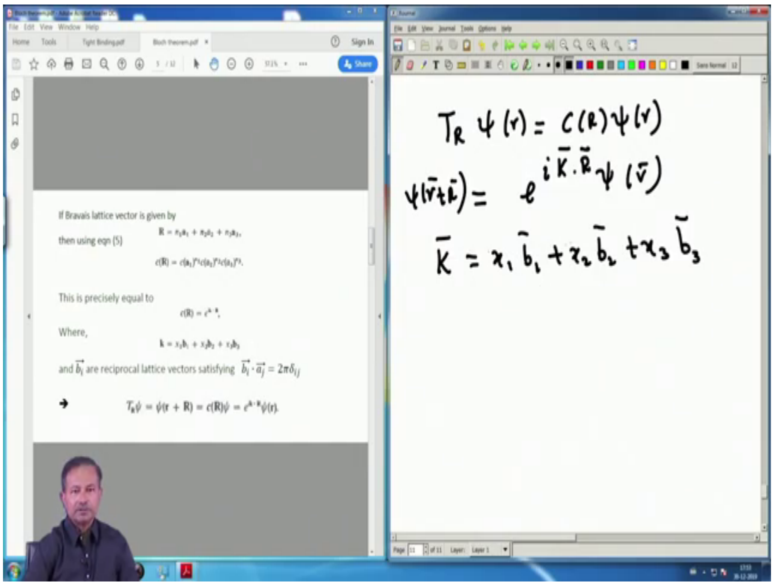
So, that means, for any c of R then you have c of a 1 to the power n 1, c of a 2 to the power n 2 are given by this R a square R is n 1 a 1 plus n 2 a 2 plus n 3 a 3, this will be c of a 3 to the power n 3, ok. But this now this if I write K equal to x 1 b 1 plus x 2 b 2 plus x 3 b 3, then where b 1, b 2, b 3 are the reciprocal lattice vectors that satisfies this relation.

This we already know this is how the reciprocal lattice vectors are defined that b i dot a i dot b j or b i dot a j must be equal to 2 pi times the delta i j. So, if i and j are equal then a this is 2 pi, if i and j are different then this is 0, that is exactly the definition of a reciprocal lattice vector b corresponding to the real lattice vectors a i, the primitive lattice vectors a i.

So, that is a suppose you would, right. Now, K equal to x 1 in to b 1 plus x 2 in to b 2 plus x 3 in to b 3, then you can easily check that this relation this relation that we got here and the previous the one c a i equal to e to the power 2 pi x i and c of R equal to c a to the power n 1, c a 2 the a 2 to the power n 2 plus c a plus 3 to into c a 3 to the power n 3.

These two, these definitions can be combined in a very small very short notation using this reciprocal lattice vector and that a short notation is simply that the wave function is T R of psi of R is c R of psi of r equal to e to the power i K dot r times psi of r.

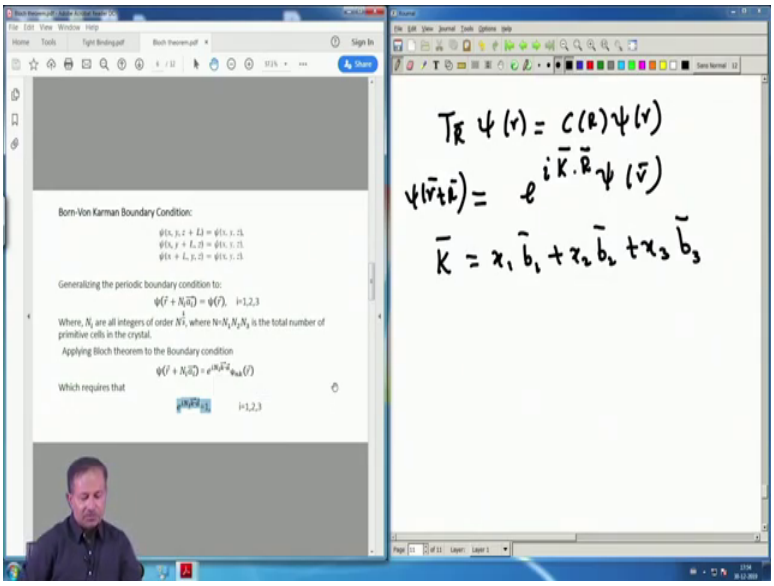
(Refer Slide Time: 22:49)



So, I now identify what the K's are K is x 1 b 1 plus x 2 b 2 plus x 3 b 3. It is a vector in the reciprocal lattice space in the reciprocal lattice, so it is. So, you have construct the reciprocal lattice of the original lattice and find the reciprocal lattice vectors b 1, b 2, b 3 and then your K is just a x 1, x 1, x 2, x 3 are integers and then it is it again belongs to the reciprocal lattice space of the all the points of the reciprocal lattice.

So, any point in the reciprocal lattice can be represented by this K and so your proof of. So, this is also equal to psi r plus R this is exactly what the Bloch's theorem said and this is the proof of Bloch's theorem that Bloch's theorem ensures that it is psi of r plus R equal to e to the power i K dot r into psi of r and the choice of K is very simple. It is the reciprocal lattice vector of the lattice the real lattice that you started with. So, that the actually completes this is a proof of the property that is in enshrined in Bloch's theorem.

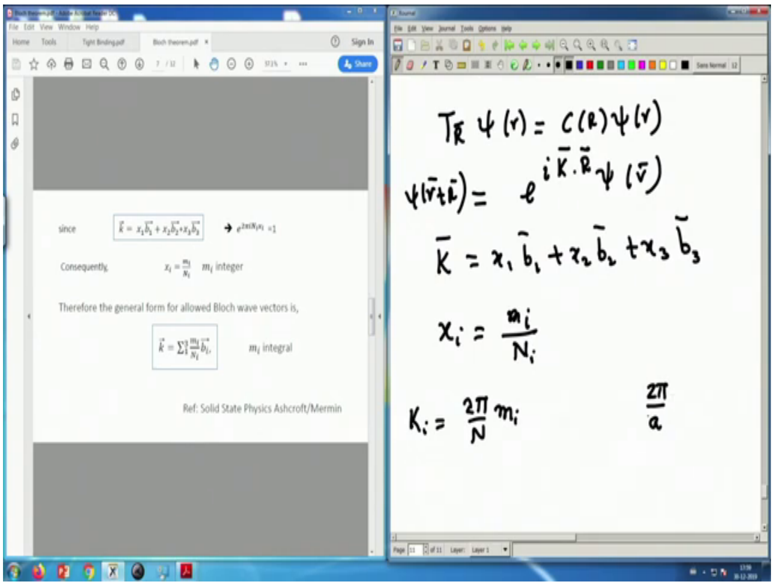
(Refer Slide Time: 24:41)



Now, of course, using this a you can remember we did this Born-Von Karman boundary conditions for a periodic lattice and using this you can find out that easily you can just see the same thing is being done here. So, basically x y and 3 directions you are putting periodic boundary conditions; with the size of the lattice is L in each direction and here for example, that is what is chosen and then this is lattice is periodic in all 3 directions and the period being L.

So, this then from the from this condition on Bloch states, you can immediately see that the solutions will have this kind of a structure, right. And capital N times K dot a equal to N whereas, i is 1, 2, 3. So, this is very straight forward this is again the exactly the same thing that we did when we did this periodic boundary condition and found out the allowed values of K and that is what is being done and this will give you the K vector in terms of this m i integers m i by N i.

(Refer Slide Time: 26:01)



So, x i are defined as then it becomes m i by N i. where N i are integers over N to the power one-third. So, N is the size of this, the capital N is the size of the nearly the number of points in each direction. So, that is the total number of primitive cells, by primitive cell one in a lattice with without a basis which is your primitive cell containing only one atom this will just be the number of atoms and if you have a basis of course, then the lattice with the basis then you have the still considered the primitive cell not the number of sides. So, that is the distinction one makes.

But this once you start doing things it will become obvious. This is not a major thing you have to remember. This is a technical point being made here that is the total number of primitive cells in the crystal not the number of points in the lattice. But this is the same as number of points in the lattice if you if you are a primitive cell contains only one atom which is what we have been starting so far except for the example of graphene which we will come back later.

For the moment you will see that N is integer. So, this N i is an integer of the order of capital N to the power one-third. But if all these N's are the same then if you have same number of atoms on each in three directions then this is the N cube, then this is again become N to the power one-third is again N. So, this line is a bit complicated, but it will become obvious as we go along, but at the moment just take N to be the number of lattice points, which is the same as being said here for a lattice without a basis; that means, one atom per even itself, ok.

So, that then gives me the value of x i and x i's are m i by N i and K is basically a sum over 1 to 2, m i by x i times b i, where m i are integer. So, that is that is exactly what we got earlier. So, you remember that 2 pi by N into integers m I of any K i. So, in one-dimension for example, this is what we got.

So, these are this is how it this is this basically is the same as the Born-Von Karman periodic boundary conditions that we obtain in our lecture during the number of allowed K values determination, ok. So, do not confuse anything this is the same as the previous K and it belongs in the reciprocal lattice vector of course, in a higher dimensional lattice.

In one-dimensional it is again a one-dimensional lattice. In two-dimension of course it is two-dimensional; it is three-dimensional that again three-dimensional, but you have to go to the you always have to remember 2 pi by see the Brillouin zone that we constructed was has a size of 2 pi by L. So, from, so K values went from minus pi by a plus pi by a. So, this is exactly what is being done here, ok. So, this is where I end the proof of a Bloch’s theorem.

Now, the next lecture we will go ahead and do the more discussions on Bloch theorem and its usefulness in giving us a solution to the Schrodinger equation or an electron in a periodic potential. And, as I said the LCO method is one fine method which does the that kind of case where you have n number of atoms, but it is as simple as what we did for two atoms. It is just extending the same theory what n number of atoms.

Thank you