Electronic Theory of Solids
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Lecture – 19
Lattice with basis: Energy Spectrum

So, we have been discussing the band structure of materials.

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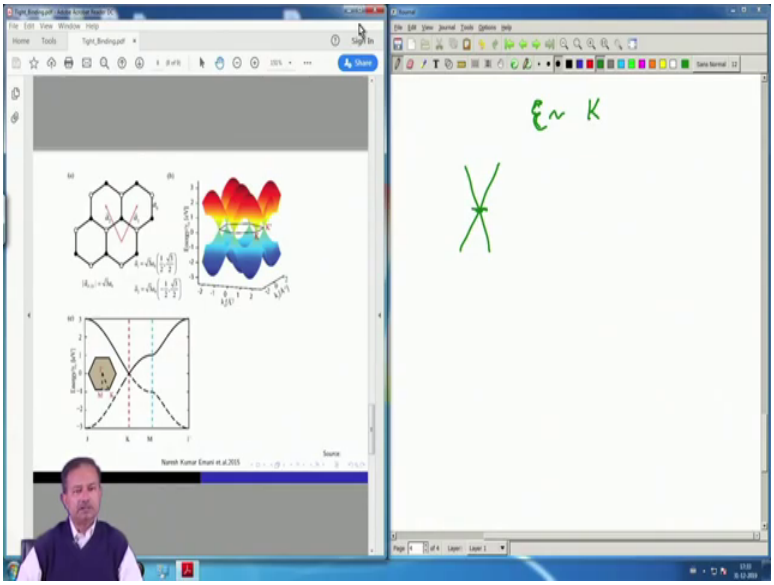

And this is a simple two dimensional system which I discussed many times now, this is graphene and this is the band structure of graphene. So, let us as I showed in the previous viewgraph.

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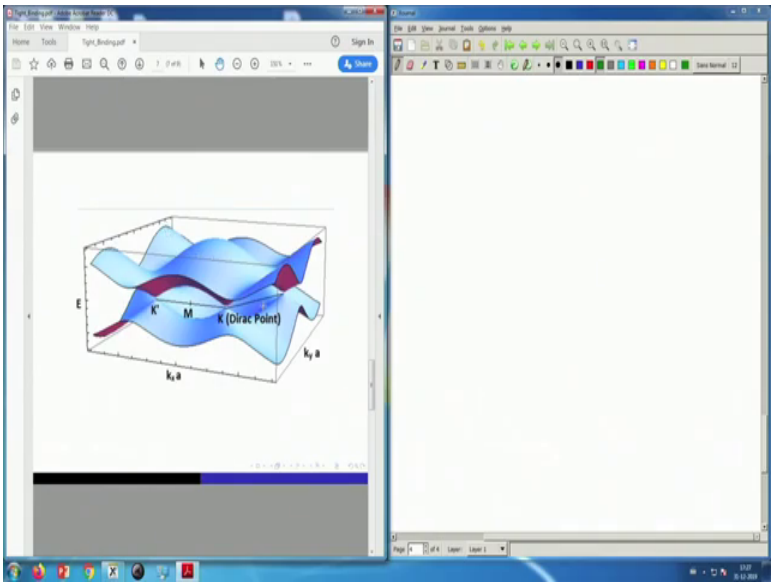

This is a E versus K x K y picture which is the same as this one. So, this is on a scale which is much compressed but, you can still see this all the points; there are 1 2 3 4 5 6 points at which the two bands touch and they touch linearly with each other, as I said the touching is like this. So, this is the these are the points at which these K and K prime points, there are 6 K and K prime points as you can easily see from here.

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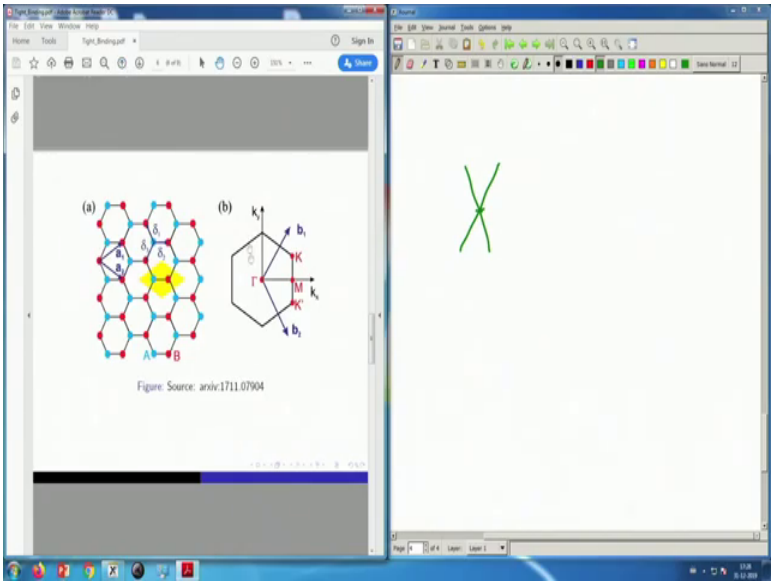

See there are 3 K points and 3 K prime points in this there are 6 vertices. So, at each of those points the band to bands touch and touch linearly. So, the spectrum here is basically E versus E goes as K ok. But, remember this is true only very close to this Fermi point ok.

So, there are 6 Fermi points; although this is it this is remember there is a two dimensional structure. So, you will only have Fermi points and you will have a Fermi line, but the line is broken up because there are only 6 places where the 2 bands touch at the Fermi surface and so there are 6 Fermi points here although it is a two dimensional system.

So, this line that is drawn is the putative line, I had these 2 bands touched along these lines that line would have been the Fermi level at half filling, but Fermi surface at half filling. Surface means a line here in two dimension. So, but that is not happening what is happening is that there are gaps in between and at only 6 points the 2 bands touch and these are the points which are the Fermi points at half filling.

So, usually the normal graphene has these 6 Fermi points. Now, the usually if you look at the band structure one actually shows it in this way. Because, in three dimension for example, you cannot show do this you have K x and Ky and energy on the other axis.

So, you only have 3 axis you can show visually. But, in three dimension you would need a K z axis as well. So, that I mean one can do, what one can do is a take sections along certain K z and still show a three dimensional plot like this. But a better way is usual the conventional way is to show the plot as shown is the lower in the lower graph. These are the symmetry direction as I said; the high symmetry directions for example, gamma M then gamma K and then K to M.

So, along these directions remember that so, gamma M, M K and gamma K these are the directions along which one plots the bands that the E versus K is plotted along these. And as you can see at K point there is a linear spectrum very close to K point but, as you go away from K this K point as you go higher up you can see that the linearity does not survive anymore, it becomes quadratic or different powers of K from linear in K.

So, linear K spectrum survives only in this region, pretty close to the K and K prime points those 6 points. So, the Brillouin zone is shown here on the left hand side along which direction the author is

plotting is also shown. So, the author is plotting along these lines dashed lines gamma M gamma M K and K gamma.

So, for example, we starts from gamma then comes to K, so, gamma to K gamma to K then K to M then M to gamma. So, it completes a full circuit; gamma K K M M gamma. And this is very usual way of showing the band structure and it actually the high symmetry directions basically tell you what the bands look like and almost all that you need to know about the band. Of course, you would like you have the information of the entire band structure at every point in the Billouin zone.

So, if necessary one can also look at those. But, usually the high symmetry directions are good enough to plot to show the nature of states and the whether there is a gap, there is a metallicity, there is a semiconductor be a conducting behavior or so on and so forth.

So, graphene for example, is like a semi metal it has only 6 points where there are 0 energy excitations available at all other points the spectrum is gaped like a semiconductor. Whereas, at 6 points it is like a metal, but that to the density of states is very very low at exactly deforming points. Because, it just touches that point as I shown like a V. Now, let me go back to how does one calculate the band structure in such a situation. So, that is lattice so called lattice with a basis ok.

So, this I will go through quickly, because this is actually a very important thing. But, this already I mean how to calculate a tide binding band structure. I have already discussed, but the special case of where when there are more than one atoms in a unit cell is important and because graphene has become so important these days one such example I will just show and then I let you work out the band structure of graphene if you want to.

So, remember the calculations that we did in which the matrix we formed was like this. Use black ink epsilon naught t 0 0 then 0, sorry then fine this is minus t.

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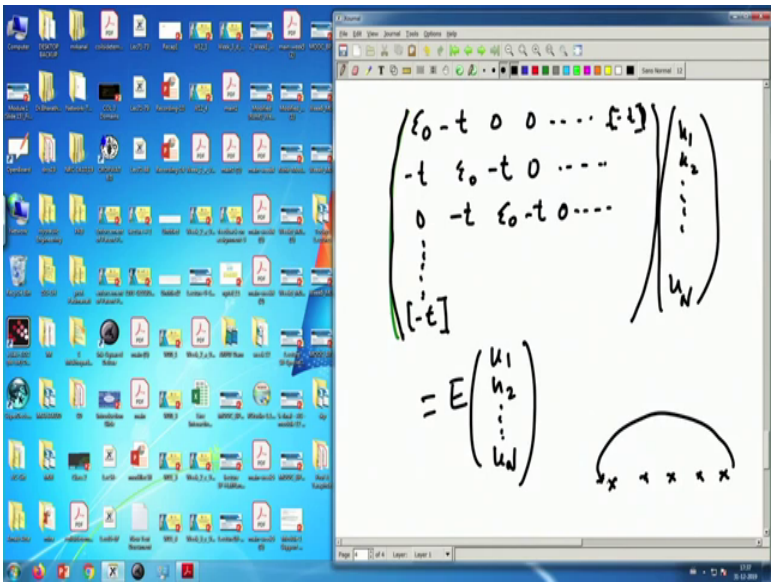

So, this is also minus t minus t epsilon naught minus t 0. It goes on 0 minus t epsilon naught minus t 0 so on and so forth. Now, there is one thing that I mentioned that if you have a periodic boundary condition. For example, you have to your first site for example, in this chain the first and fifth sides are nearest neighbour now in a periodic boundary condition because, you have to fold this back here.

So, that means this element the last element here will also be minus t if you are using periodic boundary condition, similarly the last element here will also be. So, 1 n and n 1 element will be minus t if you are using the periodic boundary condition. Otherwise, you do not have. In open boundary condition; these will all be these are all 0s.

So, this is the only difference between a periodic and a [open boundary conditions] so this one this then u 1 u 2 and so on u N equal to E u 1, u 2 u n that is the difference between the 2 cases. These terms in the square bracket exist for periodic boundary condition and they are set to 0 they are 0 basically in the open boundary condition because, in that case you do not have the last one Nth one as a neighbour to the first one ok.

So, this is how this is the matrix that we wrote down, but this is for a unit cell containing only one atom. Now, what happens if I have more than one atom in the unit cell? I will just show you briefly,

how to do this there. The same thing can be done; same Bloch theorem can be used for that case also ok.

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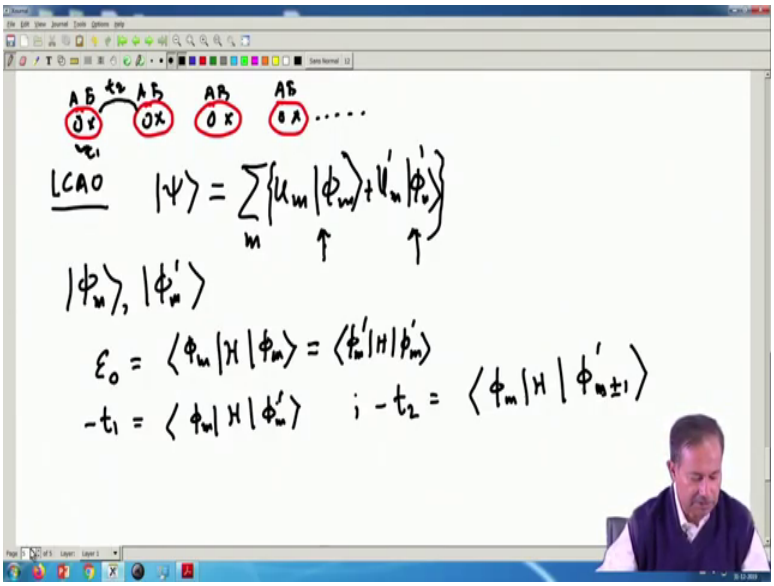

So, let me just start with a situation where; for example, I have two atoms denoted by circle and cross then circle and cross circle and cross and circle and cross and so on. So, this is so these atoms are let me call them A and B A B A B A B and so on. I will use open boundary condition for the time being, but that is just a matter of convention you can depends on the system that you want to work in.

So, this again what I do is that I will follow the same procedure that I did for the previous case. I will write down the LCAO function which is a linear combination as u m sum phi m plus u prime m phi prime m ok. This is how I will do it.

So, this what does, what am I doing? What are these two phi m and phi m prime? So, phi m phi m and phi m prime phi prime m are the orbital's that I am using from the mth unit cell. So, what is a unit cell here? See unit cell consists of these two atoms. This is one unit cell, this is another unit cell, this is one and this is one and so on. And each of these two atoms A and B contribute one orbital each. These orbital's I called phi, so from A I get phi m and from B I get phi prime m.

So, m denotes the location, this is basically the unit cell location m x unit cell, this is third, this is fourth and so on. And phi and phi prime are the two orbital's contributed by the two atoms A and B from each

unit cell. So, this is again the same prescription that I did. But of course, the matrix will now become a bit more complicated. So, let me just carry on doing.

So, again I will do the same variational principle and actually without even doing that calculation one can write down the structure of the matrix. Now, there are two kinds of so called hopping integrals which gives me which earlier gave me minus t. One hopping happens between the two atoms a and b here right in the same orbital the another hopping that happens is it happens between this A and B orbital's in the nearest neighbour unit cells.

So, there are two kinds of hoppings that one has to take care of. And since, I am only bothered about the nearest neighbour hopping I will not bother about x x hopping or o o hopping A A hopping or B B hopping for example. So, the there are only two kinds of hopping, I will call them t and t prime. So, t is in within the unit cell, so t I let me call them t 1 and t 2. Because, then there is no confusion with this prime. So, there are two kinds of hopping. So, let me write down these integrals. One integral is the epsilon naught which is phi m.

So, let me not write it sorry phi m H phi m ok. So, this I called the hopping, I also take these to be same, but it is not necessary that I have to take it to be the same, but for convenience because the matrix I want to and to let then I want to I want the matrix to look simple. So, let me just take this to be the same as phi prime m H phi prime m I could as well take this to be some epsilon naught prime hardly matters ok.

So, because I have graphene in mind actually because in graphene the two sides are not different atoms, but they are the same atom in equivalent position. So, for them for in that case this is true that both of them being carbon atom you can this epsilon naught is the same for phi and phi prime ok. But, as I said I can as well choose them to be different there is no problem in that ok.

There are other quantities which is say minus t 1 which is equal to phi m H and t 2 is phi m H phi m prime m plus or minus 1 ok. So, what does it as in my previous picture I showed? I can show you what I am doing. So, this is remember this I now basically called t 1 the hopping between these two and this hopping I called t 2 minus t 1 and minus t 2.

So a hopping between the atoms in the same unit cell is called look at this t 1 is the m th unit cell, the phi and phi prime on both sides of H. Whereas, t 2 is mth and m either on the right or on their left m plus minus 1 these say between different unit cells and that is that I called t 2.

And as I said there is no inter unit cell where both sides are either phi m or phi m prime. Because, I have not I am not considering any hopping between B and B and A and A at different lattice a different unit cells ok. So, let us then write the matrix straight away. So, how do I write for the basis? They look at the basis; the way to write the basis is exactly the same.

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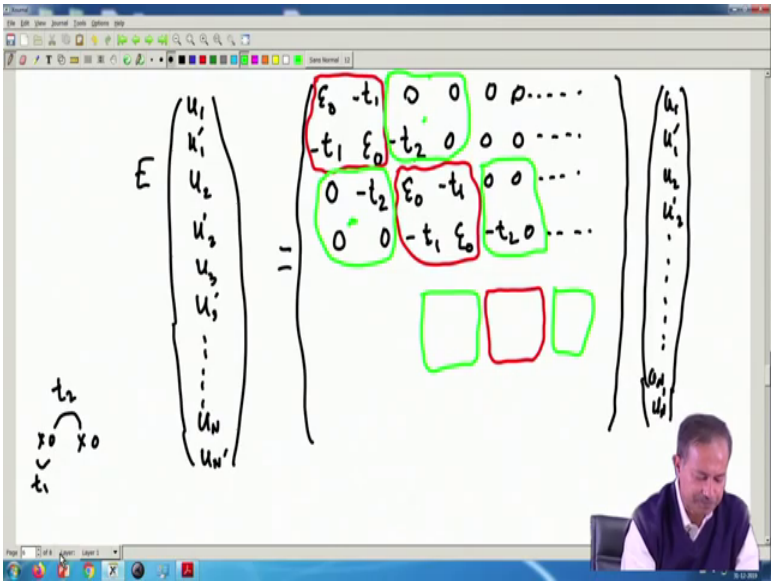

So, E times u 1 u 1 prime, remember I let me just show you what I did. So, these u m and u prime m, so these are my coefficients. So, I will write the basis in terms of these coefficients. And each m will give me two coefficients ok. So, that is what I am doing. So, u 2 u 2 prime u 3 u 3 prime and it goes on up to u n u n prime, for a finite system.

So, this is my basis ok. So, what will be the matrix? I will find out the matrix. So, again the same basis is will be written here; u 1 u 1 u prime 1 u 2 u prime 2 and so on; u n u prime n ok. So, now, I have to construct the matrix. One thing is very simple that the diagonal elements, because of my choice; the diagonal elements are all epsilon naught. Now the next element is between what? Between u 1 and u 1 prime.

So, that is between phi m and phi m prime Hamiltonian matrix element, which I know is minus t 1 ok. For the first site there is nothing else and so, I will just continue doing this for the second the interesting thing is so, this 0 0 0 0 goes on. I am using open boundary condition. So, I will not have to bother about the one nth 1 2 nth coefficient the matrix element. So, the next one is again epsilon 0, but now let us see what is the situation. So, this was my arrangement.

So, this is t 1 between the two and between these two is the t 2, minus t 1 and minus t 2. So, that one t 1 for the first one I have already used. So, but for the u 1 prime which is for this B site, I have a t 2 also it is to the next site. So, on the right hand side I have a t 2 on the left hand side I still have this t 1. So, on the right hand side; I now have t 2.

Now, one thing is actually very simple because the Hamiltonian is Hermitian matrix, you actually need to only find one side of this diagonal. Diagonal elements and one side of it the other side can be easily constructed by the property of hermeticity. So, for a real system; that means the symmetric matrix.

So, if I have t 1 here, minus t 1 here as 1 2 element, then 2 1 element has to be minus t 1 again. For example, here I have 2 3 element minus t 2; that means, 3 2 element has to be minus t 2 again and so on and so forth. So, the rest are all 0s then again as I said the I will write epsilon 0 here. Now 2 3 element is minus t 2. Then 3 2 element will also be minus t 2 and on that side I will have t 1 minus t 1 and so on ok. So, this is the structure of this matrix it looks a bit complicated, but it is actually not.

So, if you look at this matrix it has certain elements certain things which repeat. So, let me show you what repeats. So, now, let us see this is 0. So, the fourth one will have epsilon naught here. On its left hand side I must have t 1, because this 1 was t 1 remember 3 4 was t 1. So, 4 3 must be t 1 and this will be minus t 2 and it goes on like this. Now look at the structure of this matrix this motif these four elements repeat along the diagonals and these let me write in a different ink these 4 are repeating along the off diagonals. And this will carry on; remember this one will come here.

So, this is again a green one, there will be a red one here, there will be a green one here on both sides and so on. But, this green one and this green one are slightly different see this green one and this green one are slightly different in the sense that one is the transpose of the other. So, these 2 by 2 matrix; if I

write this as a 2 by 2 matrix and this other one has to another 2 by 2 matrix they are just transpose of each other. So, that is all I have to remember.

So, then the next view graph I mean next calculation that I can do is very straightforward I can write this as a similar equation as I did for the one site per unit cell case. And I will just write it down, but now the elements that I used there they were just H 1 1 H 1 2 this kind of elements, t epsilon naught t minus t and so on, now those will be matrices.

So, the matrices are which one the ones that I encircled in red and the ones that I encircled in green. So, let me write down then you will see how it works out. So, let me write a matrix let me redefine and write a matrix as beta equal to this is just a notation.

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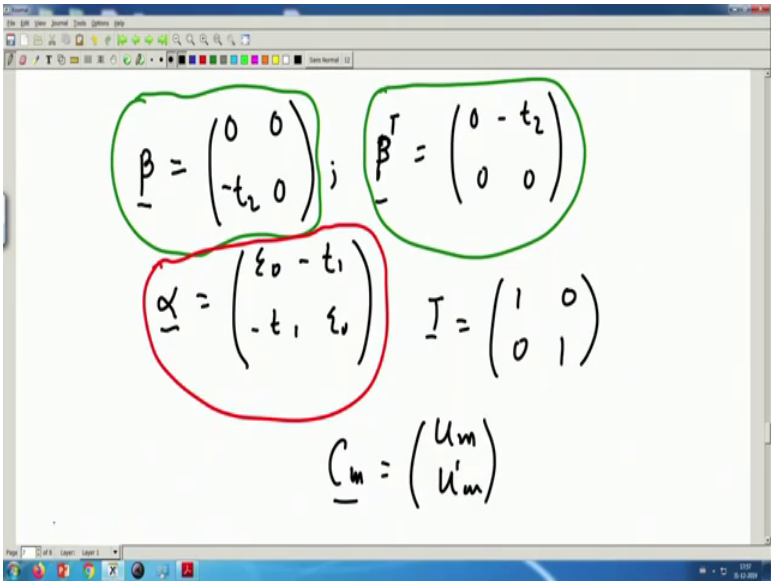

I am just using a notation, I am writing I am calling it beta is 0 0 minus t 2 0. Do you remember this under I am putting on a line under to just to denote that it is a matrix.

So, beta under with an underline means that it is a matrix. Just to remind myself. Then beta transpose this matrix is simply 0 minus t 2 0 0. So, beta transpose is just this matrix ok. And I have the other matrix which I let me call it alpha which is the matrix that I know which is epsilon naught minus t 1 minus t 1 epsilon naught.

So, remember these. So, let me go back one page. So, remember these epsilon naught t 1 minus t 1 minus t 1 epsilon naught this is the red 2 by 2 matrix the and the green 2 by 2 matrix on the upper right is 0 0 minus t 2 0 which I called beta and this lower t 2 matrix lower matrix is 0 minus t 2 0 0 this green one; that means, it is just the transpose of the upper right one ok.

So, that is what I have done. So, remember these were my green matrices, one is the transpose of the other and this is my red matrix 2 by 2 matrix. Of course, I will also use the identity matrix which is simply I equal to in two dimension 1 0 0 1 that also I will use ok. So let me just now write down the equation the same matrix equation now I can write as ok. So, let me define one more quantity which is C m which is u m and u prime m. So, this is a 2 by 1 vector.

So, I will write everything now in terms of these objects any underline means it is a vector. So, I for example, is a 2 by 2 identity matrix ok. So, let me just write down the equation.

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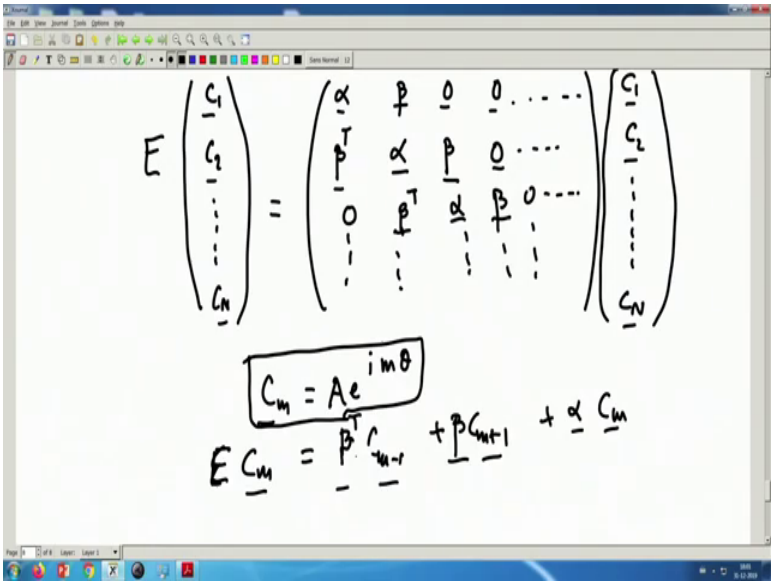

E times you can check for yourself, multiply and check for yourself will be c 1 c 2 c N equal to alpha beta then all 0 s, but these 0s are also 2 by 2 matrices remember they are 0 0 0 0, four 0s. And then beta transpose alpha, beta, then 0 these 2 by 2 0 0 0 0 matrices. This goes on and then, so then again here a beta transpose alpha beta and then 0s and so on times this vector c 1 underscore underlying c 2 underline c N underline. All these are these 0 underlined is a 2 by 2 zero matrix.

Then again do the same thing exactly the same, then I write this matrix C m equal to A e to the power i m theta as before. So, I can write this, so take any m th column of this suppose I just an m th column. So, that m th column now reads like E C m underscore, equal to C m minus 1 underscore, beta transpose underscore plus C m plus 1 beta underscore plus alpha underline C m ok. So, that is the sorry I should write it on the right hand side.

So, these are matrices. So, I should write this beta transpose C m minus 1 beta transpose and beta C m plus 1. So, that is the matrix equation that 1 has obtained it is a 2 by 2 matrix equation which one has to basically solve and the way to solve it as I said I will exactly do what I did. I will use a solution which is consistent with Bloch's theorem.

So, what I will do is that I will show it in the next class and find the spectrum for you and show you, how such a simple generalization works beautifully to calculate the energy spectrum for systems with more than one atom per unit cell. Here of course, I have taken only two, but that can again be generalized to a larger number of atoms in the unit cell.