Introduction to Solid State Physics

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Lecture – 59
Mixing of plane waves to get Bloch wavefunction – II

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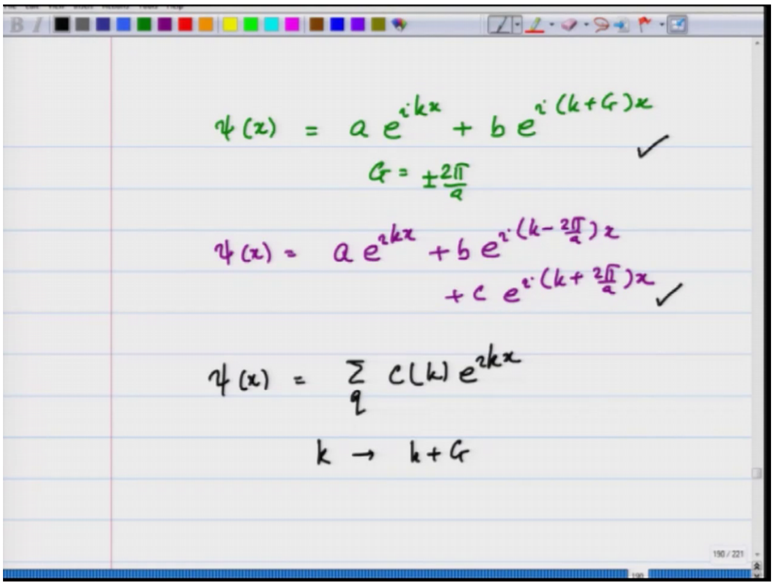

In the previous lecture I took psi x to be a e raised to i k x plus b e raised to i; k plus G x, where G was 2 pi by a plus or minus and showed how I can get energy bands or energy gaps. Then I also showed you if I take psi x to be equal to a combination of three plane waves e raised to i k x plus b e raised to i k minus 2 pi by a; x plus c e raised to i k plus 2 pi by a; x how I can get 3 bands? And this I will also give you as an assignment problem.

Now, we generalize this and think of what happens if I take psi x to be a combination of many many many different case. How do these plane waves couple from the two exercises that I have just mentioned? You can see that k will couple with k plus G where G could be 2 pi by a, 4 pi by a, minus 2 pi by a minus 4 pi and so on. However, now we are going to prove it and this is also lead to another proof of Bloch's theorem. So, let us look at the Schrodinger equation.

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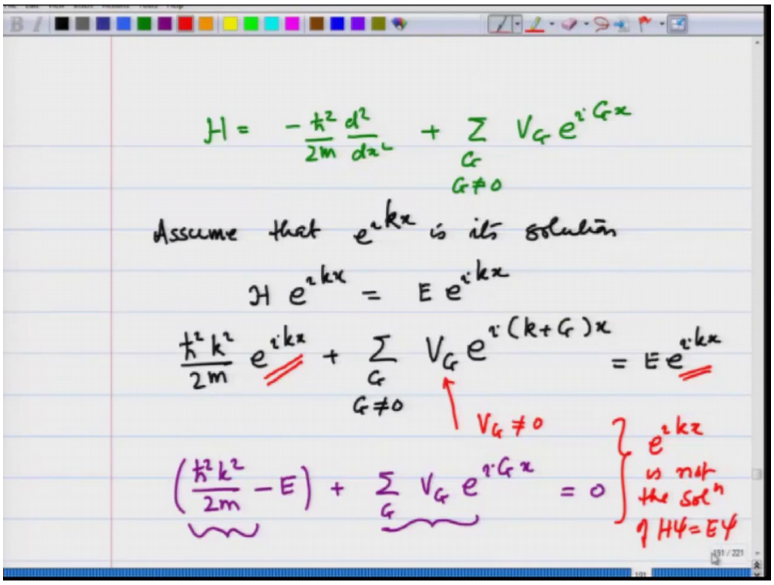

H the Hamiltonian is minus h cross square d 2 by d x square over 2 m here plus summation G and we have taken G not equal to 0 V G e raised to i G x. Assume that e raised to I; k x is its solution and substitute it in the Schrodinger equation. So, I take H e raised to i k x is equal to E, e raised to i k x; then I find that I have h cross square k square over 2 m, e raised to i k x plus summation over G; G not equal to 0; V G e raised to i, k plus G x is equal to E e raised to i k x.

What you notice is because of these V G's not being 0 this equation cannot be satisfied because I have e raised to i k x on this side, e raised to i k x on this side which I can cancel from the two sides. And then get h cross square k square over 2 m minus E plus summation G; V G e raised to i, G x is equal to 0. This is a constant; so it tells you either the potential itself is 0 and in that case e will be equal to H cross k square over 2 m; if potential is not 0 then this equation certainly is not satisfied.

And therefore, we have to do something e raised to i k x cannot be the solution. So, we conclude from here that e raised to i; k x is not the solution of H psi equals E psi or the Schrodinger equation.

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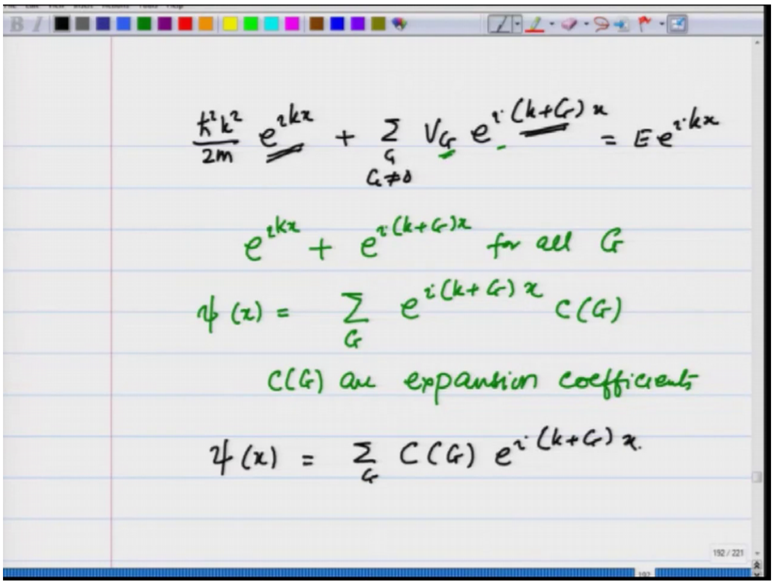

So, what did we have? Let us rewrite it; h cross square k square over 2 m e raised to i k x plus summation G; G not equal to 0, V G e raised to i k plus G x equals E; e raised to i k x. What you notice is that when I have this e raised to i k x here the other terms i k plus G also popping they start coming in.

So, if I want to satisfy this equation on both sides; what I should have is for each e raised to i k x, I should also add to it e raised to i; k plus G x for all reciprocal space vectors G. And therefore, I should take the solution psi x to be equal to summation over G; G equals 0 is now included e raised to i k plus G x C G; where C G are expansion coefficients.

And notice with k I am adding only i, e raised to i k x I am adding only e raised to i k plus G x because of this specific nature or periodicity of the potential. I cannot add anything else if I substitute anything else here, again the equation will not be satisfied. So, now let us substitute this n and see what we get. So, I am going to get the wave function psi x which is equal to summation G, now G equals 0 is included C G e raised to i k plus G x.

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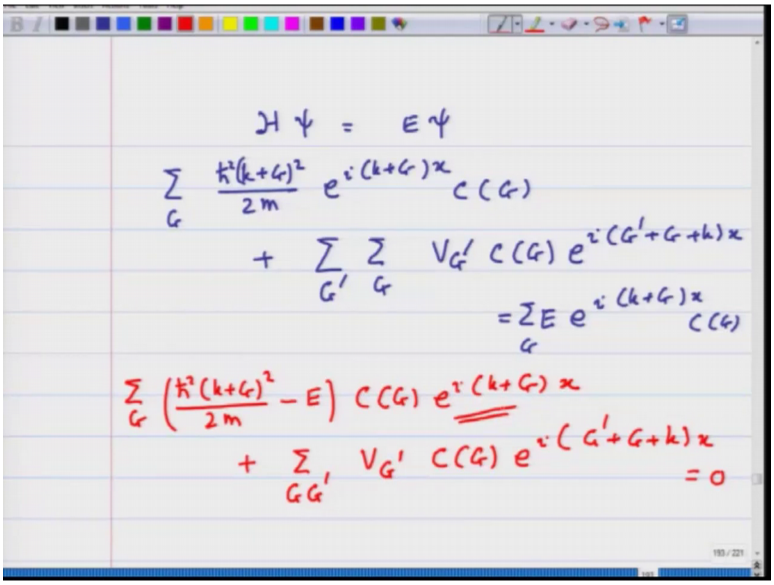

And when I substituted this in H psi equals E psi; I am going to get summation G h cross square k plus G square over 2 m e raised to i; k plus G x, there is a C G here plus for the potential I have to now write G prime; summation G V G C G e raised to i; this is V G prime, G prime plus G plus k; x equals E e raised to i k plus G x C G summed over G; these are different terms.

So, now let us bring everything to the left hand side. So, I am going to get summation G h cross square; k plus G whole square over 2 m minus E C G; e raised to i k plus G x plus summation over G; G prime V G prime; C G e raised to i; G prime plus G plus k x is equal to 0. Let us now equate the coefficients corresponding to each e raised to i; a plus G on both sides.

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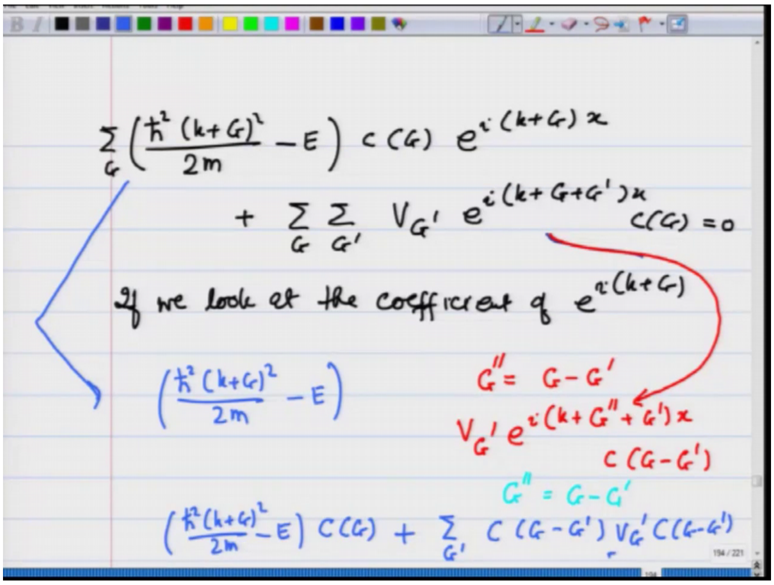

So, this equation is h cross square k plus G square over 2 m minus E C G e raised to i k plus G x plus summation over G, summation over G prime V G prime e raised to i k plus G plus G prime x; C G equals 0; this is also a summation over G.

If we look at the coefficient of e raised to i; k plus G; then in the first term this term it is h cross square k plus G whole square over 2 m minus E. And in this term the second term the G; they will appear would be actually I want e raised to i k G x and therefore, I should have G equals the term that will be picked up will be let me call it G double prime equals G minus G prime.

So, that I will have V G prime e raised to i; k plus instead of G, I should have G double prime plus G prime x C; G minus G prime where G double prime is G minus G prime. So, I get the equation h cross square k plus G square over 2 m minus E; C G plus summation over G prime, C G minus G prime V G prime. And all these give me the coefficient C; G minus G prime and e raised to i k G x; for all G prime, so any G prime I can pick G minus G prime as G double prime right.

So, then this should all be 0; let me rewrite this whole thing.

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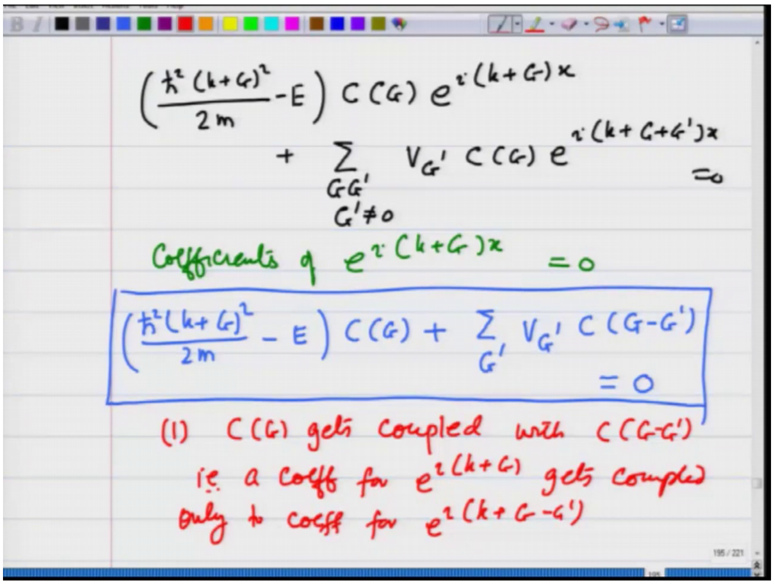

The equation I have is h cross square k plus G whole square over 2 m minus E; C G plus summation over G and G prime V G prime; keep in mind the G prime is not equal to 0; C G e raised to i k plus G plus G prime x is equal to 0, here is e raised to i k plus G x.

Now I want because these are all independent functions e raised to i k x; I want the coefficient of e raised to i k plus G x to be 0. And therefore, I am going to have h cross square k plus G whole square over 2 m minus E; C G plus summation over G prime; V G prime. For each V G prime I pick up a coefficient C; G minus G prime and this is equal to 0. This is the equation that determines coefficient C and C G minus G prime.

You notice one thing here that C of G gets coupled with C; G minus G prime. That is a coefficient for e raised to i k plus G gets coupled only to coefficient for e raised to i k plus G minus G prime; that is the k which is displaced by it from it by another lattice vector.

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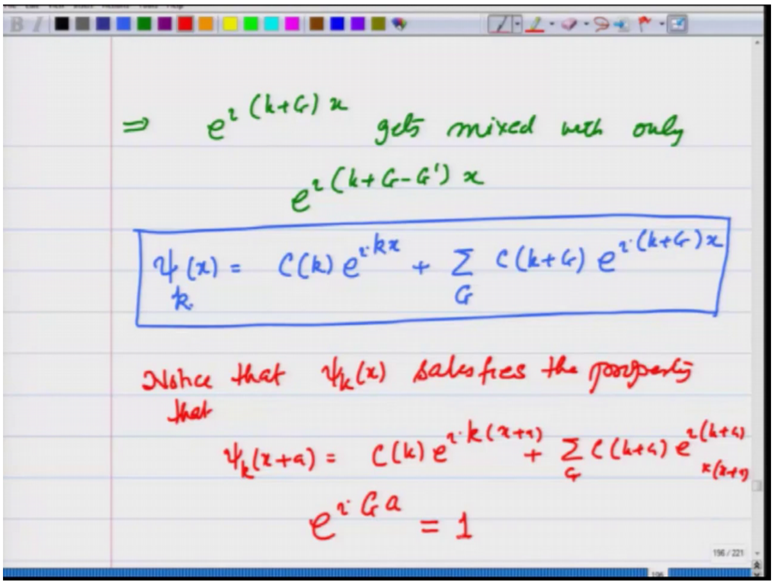

This implies e raised to i k plus G x gets mix with only e raised to i k plus G minus G prime x.

So, only those plane waves mix that have a difference of G prime that is another lattice vector form each other. So, the wave function is going to be psi x is equal to; let me now separate out G equals 0. Some coefficient C k; e raised to i k x plus summation over G. Now I am going to label it as C k plus G; e raised to i, k plus G x. Earlier I had not written C k it was just C g; so k was C 0 and then C G; now I am specifically writing this k because k gets mixed only with k plus G not any other k.

So, I can actually label this wave function as being specified by k. These are the wave functions and notice that psi k x satisfies the property that psi k; x plus a is going to be equal to C k; e raised to i k x plus a plus summation over G, C k plus G e raised to i; k plus G times x plus a. Now e raised to i G a is equal to 1.

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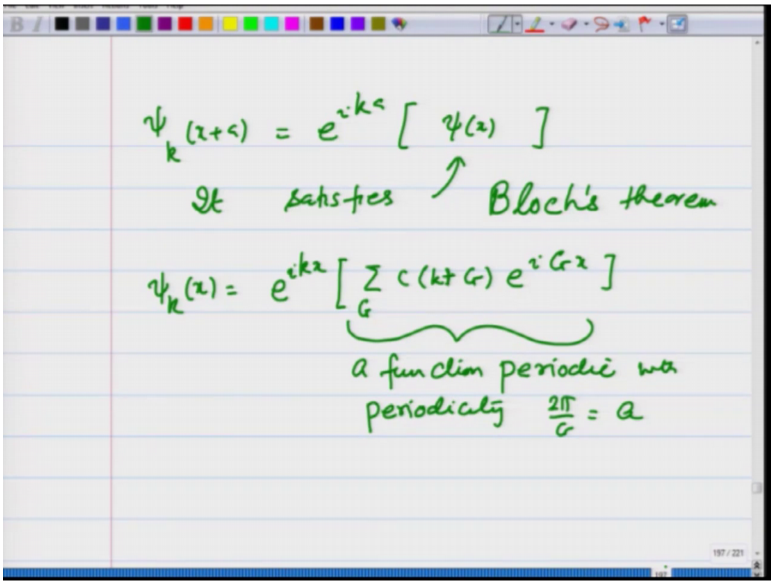

Therefore psi k x plus a becomes e raised to i k a times whatever that summation is left is psi x.

So, it satisfies this property and that is Bloch's theorem. You can also see that I can write psi k x as; if I take e raised to i k x out I have summation. I can write this as G all G's included k plus G e raised to i; G x, G equals 0 is also included because C k is included here and this is a function periodic with periodicity 2 pi over G which is a; so, this is another way of writing the Bloch's theorem.

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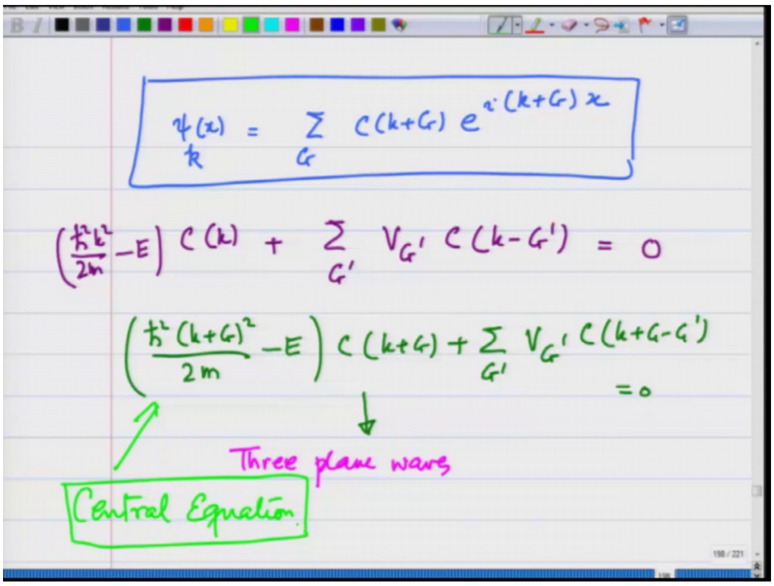

So, what we found is that when I turn this periodic potential on the wave function is of the form it can be labeled by a k equals summation I can now write G; G equals 0 included C k plus G e raised to i k plus G x. And C k satisfies C k h cross square k square over 2 m minus E plus summation G prime; V G prime C k minus G prime equals 0, this equation can also be written for each other C k g.

So, I can write h cross square k plus G square over 2 m minus E; C k plus G plus summation G prime V G prime C k plus G minus G prime is equal to 0. Again at G prime equals C the C k will come here. So, this is a set of equations for all Cs and if you want to now calculate the energy, you have to take a finite number of these equations and diagonalize; the resulting determinant for the coefficients of Cs and that leads to the bands. Example of this we have already done three plane waves, were mixed and you got a model for the calculating energy in the previous lecture. I can mix 4, 5, 6 whatever number and then make a determinant and solve it.

So, this is the way the band structure is gotten by mixing plane waves this is the way that Bloch's theorem is also proved this by the way is known as the central equation.

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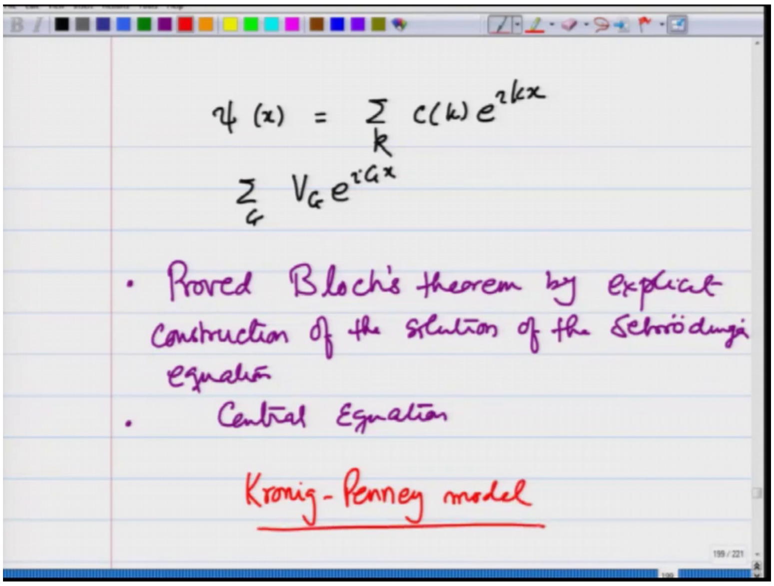

Some of the books also bring this equation by writing psi x as summation over all k; C k e raised to i k x substitute this in the Schrodinger equation and then bring the same equation back realizing that V G e raised to i G x summation over G is the periodic potential and therefore, only k and k plus G and all those terms come into the picture.

So, what I have done in this lecture is proved Bloch's theorem by explicit construction of the solution of the Schrodinger equation. And also as a result got the central equation which when diagonalized gives you the energy eigenvalues or depends; in all this we have to solve a determinant which is of finite order.

Now, infinite order, but we have to make it finite; in the next lecture I am going to solve a model which can be solved exactly to obtain the energy structure and in this model which is known as the Kronig Penney model. And that can be solved exactly and you will see how it leads to energy bands and so it gives a good idea about what happens when electrons move in a periodic potential. So, I will stop this lecture here next lecture we solve Kronig Penney model which is an exactly soluble model.