Introduction to Quantum Mechanics
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Lecture - 03
Kroning-Penny model and energy bands

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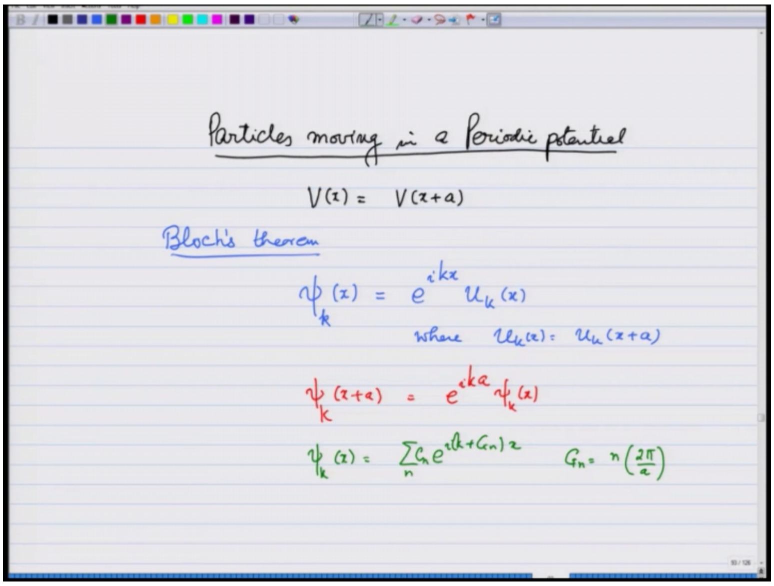

In the previous lecture we started our discussion on particles moving in a periodic potential. That means, the particles are moving in a potential which is periodic with periodicity a and we have confined ourselves to discussing one dimensional cases. And what we discussed was in these cases the wave function satisfies Bloch's theorem that says that a wave function psi x and I will label it by k has the form e raised to i k x u k x where u k x is also periodic function, the same periodicity as the potential.

This is also expressed in a different manner by writing that psi k x plus a is always psi k a e raised to i k a psi i k x. And third form that we wrote this as was that psi k x can be written as summation n e raised to i k plus g n x and there are some coefficients C n's where g n is n times 2 pi over a. So, these are three different forms that this wave function comes in, and what does it mean? What are the consequences of having a wave function like this?

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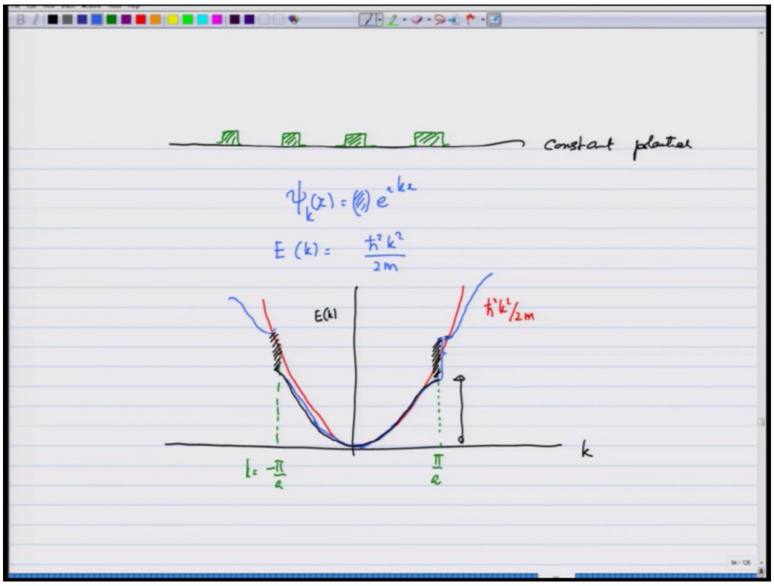

So, what happens, I will just tell you first and then show this through examples. Suppose I have a potential which is constant. In this case what happens is that the wave function psi k x is e raised to i k x with some normalization here and the energy of the particles e k is given as h cross square k square over 2 m. So, if I would plot energy versus k, e k versus k it would look like a parabola here, this is h cross square k square over 2 m.

If I now introduce this periodic potential and let me introduce it like bumps at regular intervals of a, the wave function takes the form of Bloch's wave function. And I can describe the energy confining myself to between k equals minus pi by a to pi by a. Now what happens now when you introduce this potential because of this particular form of the wave function, the energy diagram becomes like the parabola initially and then it changes near pi equals a it changes and becomes like what I have shown through blue colour, and after this again there is a change.

So, there is a range of energy which I will now black out where no state exists there is no state that is this year. So, what you get is a band of energy, energy ranging from 0 to up to this band all the energies are in this band and then there is a gap and then the energy again picks up is in the next band. And the way you show it is since we said that all k's within k plus g r equivalent. So, I shift this band here and bring it in.

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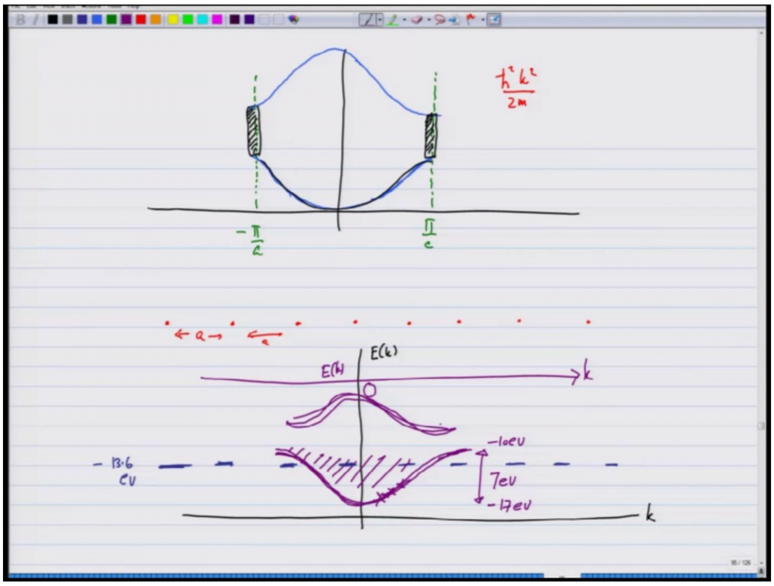

So, what we started with was the energy diagram for a free electron gas which was h cross square k square over 2 m, and then when we introduced that periodic potential I can now confine myself between minus pi by a to pi by a, the energy fell into this band.

Next level of energy is like this, but as we said we can always bring k back to within this zone (Refer Time: 05:36) zone and the next band then would look something like this. So, I will erase this portion here, raised this line up. So, for each k there is a band of energies and then the next band and then next band and so on. So, this is what happens when I disturb this free electron gas.

So, there are these gaps which open up which I have show by this black portion where no state exists, these energies cannot be taken up by the particle and the particle can take any energy in this band; first band second band and so on you may ask why did I start with free particles, I could have started with atoms. For example, if I have atoms like searing on regular interval a then I know that each atom has an energy at a fixed value.

For example, for hydrogen atom it will be minus 13.6 e v, each atom has this. So, where is the band coming in from? Or what does the Bloch equation do? What happens now if I would do plot the energy. So, I will again make this picture e k versus k and show that these energy is now are going to split and make a band. So, what happens now is let me now because the energy is negative start from e equals e k 0 here and this is k this is k e equals 0 here. What you will see that all these energy levels now with respect to k again form a band. And this energy is going to be negative. So, it is not minus 13.6 rather it is over this band which could be spread around minus 13.6. Let us say for example, it could be say from minus 17 e v to minus 10 e v

So, this is a band of seven electron volts which is formed all the energy levels that were there are going to fall in this. So, there is an energy level here, energy level here, energy level here for as a function of k. Notice that Bloch's theorem said that wave function depends on k which is a quantum number that specifies the state. It is also a good quantum number because there is a symmetry it is involved with that symmetry, but it did not say that energy has to be positive.

In the free electron case when I disturb them by a regular potential the parabola breaks up. In the case where atoms are there the all the energy levels that were there separated at minus 13.6 they form a band and then there could be next band formed by the next exile state energy and so on.

So, what happens is a form, the energy is in the form of a band and they have consequences. So, first now let me show you the formation of this band through a model called the Kronig-Penney Model.

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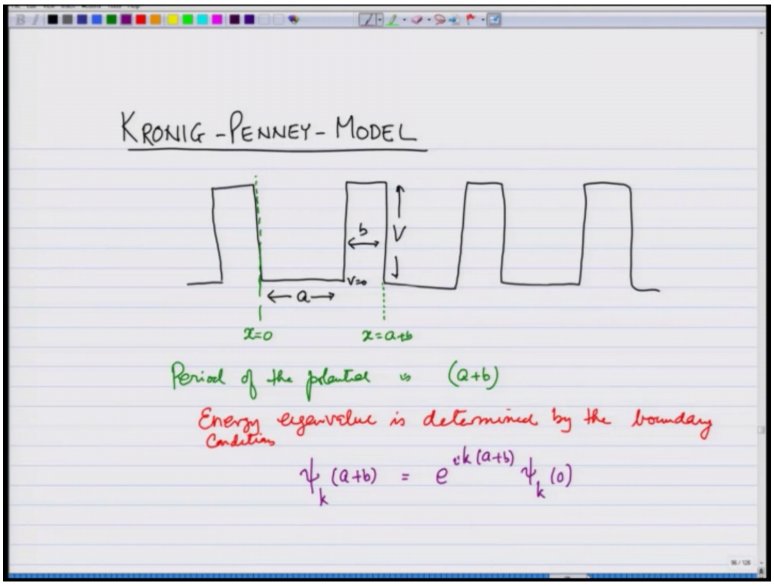

What we consider in this case is that the potential is a collection of these barriers. I would earlier, what I want to show is that this leads to bands. So, let us say this distance is a and the barrier is of width b, the height is v and here v equals 0 at the bottom. The wave function I know is of the Bloch form. This point at one edge of the potentially I am going to take as x, the point here shown by green is x equals a plus b and then the potential repeat itself.

So, periodicity period of the potential is a plus b. How do I calculate the energy for each k? Now recall in earlier cases at energy Eigen value is determined by the boundary conditions. So, in this case also we are going to apply the boundary condition. Our boundary condition is going to be provided by the Bloch's theorem. So, what we are going to say as that wave function psi k at a plus b is going to be equal to e raised to i k a plus b times wave function psi k at 0 and this should lead to the energy eigen value as I am going to show now.

We are going to assume that the energy lies below v. So, let me make it again, the potential looks like.

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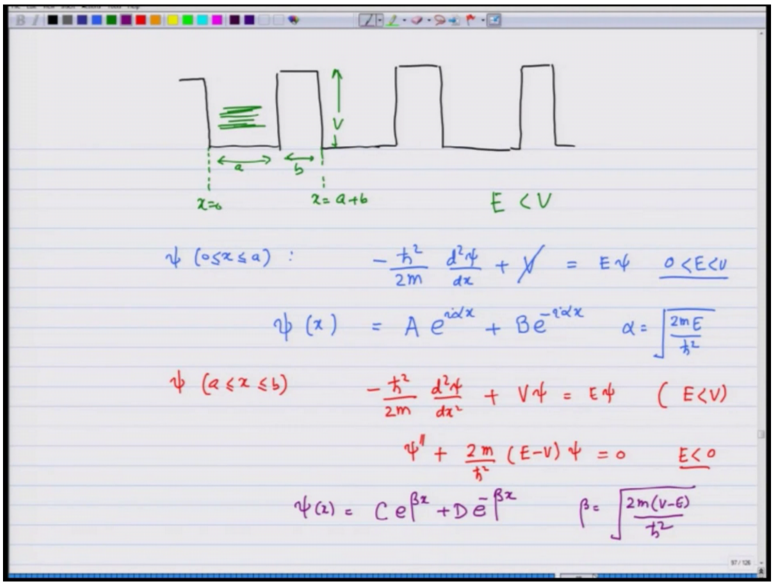

What I am showing now on your screen with widths being a here and b here on the left is x equals 0, this point is x equals a plus b the height is v. And we are going to assume that all energies we are considering are below v. So, we are considering e is below v. If e is greater than v you can again right the same condition, but right now am just taking one particular example.

So, now wave function psi for x between 0 and a is determined by the Schrodinger equation minus h cross square over 2 m d 2 psi over dx square plus v which is 0 is equal to e psi. So, e is less than 0 or e is less than v, but is also greater than 0. So, I get psi for x between 0 and a equal to e raised to i alpha x times the coefficient b a plus another coefficient b e raised to minus i alpha x where alpha is square root of 2 m e over h cross square e is greater than 0. So, there is no problem, this is like that.

Now, for the region psi x between a and b wave function is given by the Schrodinger equation minus h cross square over 2 m d 2 psi over dx square plus v psi equals e psi. And we are taking the case where e is less than v if e is greater than v all you have to do is make a slight change from the hyperbolic function you want to get a trigonometric functions, but that is a trivial case.

So, I can write this as psi double prime plus 2 m over h cross square e minus v psi equals 0 and since e is less than v i get the solution psi x equals some C e raised to beta x plus D e raised to minus beta x where beta is square root of 2 m v minus e over h cross a square. So, keep this in mind that alpha and beta given like this.

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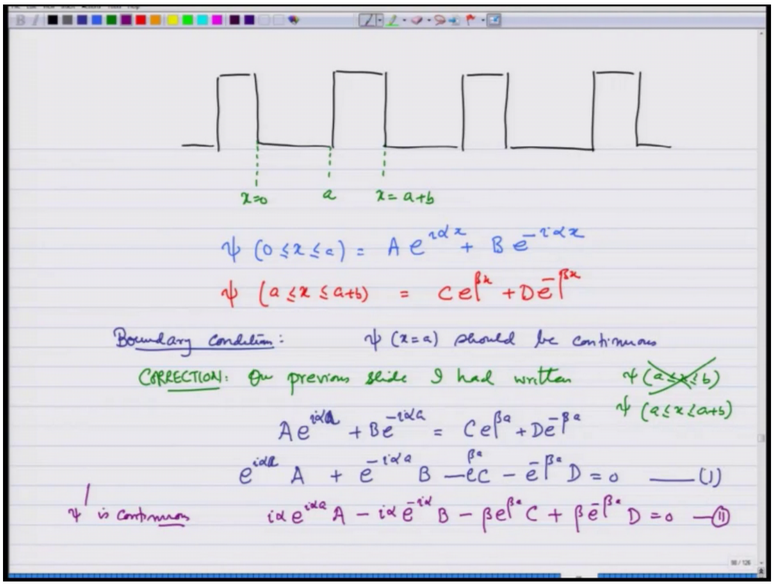

So, what I have now is I will again make this picture of this potential, x equals 0 here x equals a plus b, this is a. What I have is that the wave function psi between 0 and A is e raised to i alpha x plus B times e raised to minus i alpha x and psi for x between a and a plus b is equal to C e raised to beta x plus D e raised to minus beta x.

Now, the boundary condition I have now unknowns A B C and D and the energy itself. Now let us apply boundary conditions. We get that psi at x equals a should be continuous, just a correction on previous slide I had written psi x between a and b that was not correct, it is actually psi between a and a plus b this should be correct. I have corrected this in in read out here.

So, now this boundary condition tells me that a e raised to i alpha a plus b e raised to minus i alpha a is equal to C e raised to beta a plus D e raised to minus beta a which I can write as e raised to i alpha a times a plus e raised to minus i alpha a times b minus C e raised to beta a minus e raised to minus beta a d equals 0, that is my equation 1.

I also know that psi prime is continuous and that immediately gives me i alpha e raised to i alpha a a minus i alpha e raised to minus i alpha b minus beta e raised to beta a C plus beta e raised to minus beta a d equals 0, that is my equation 2. I should have an a out here.

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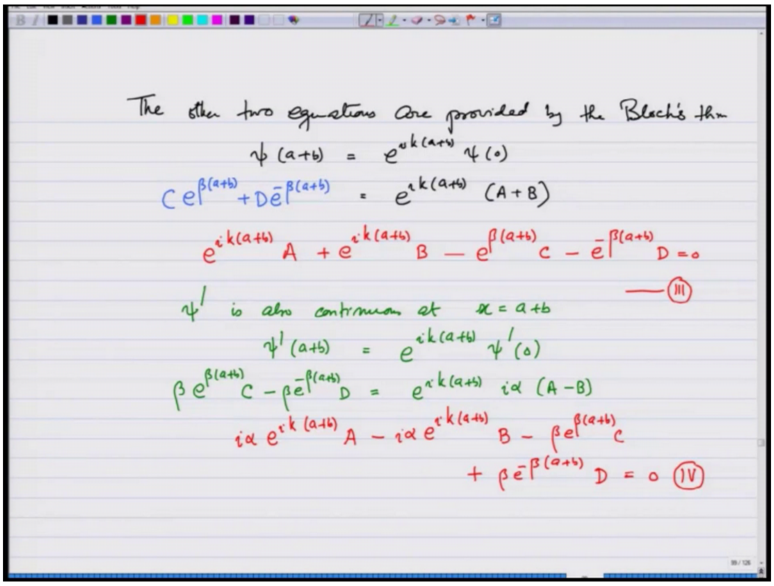

So, I have gotten two equations, still there are four unknowns. The other two equations are provided by the Bloch's theorem which says that psi a plus b should be equal to e raised to i k a plus b psi at 0. And psi at 0 I know is a plus b and psi of a plus b is nothing but C e raised to beta a plus b plus D e raised to minus beta a plus b.

So, I get the equation from here that e raised to i k a plus b times a plus e raised to i k a plus b times b minus e raised to beta a plus b times C minus e raised to minus beta a plus b times d is equal to 0, that is my equation number 3. And finally, equation number 4, since psi is continuous, psi prime is also continuous at a plus b, psi prime is also continuous at x equals a plus b.

So, I am going to have psi prime at a plus b is equal to e raised to i plus b psi prime at 0. Which gives me e raised to i k a plus b psi prime here is i alpha a minus b. And on the left-hand side I am going to get beta e raised to beta a plus b times C minus beta e raised to minus beta a plus b times d equals this.

So, this equation now becomes i alpha e raised to i k a plus b times a minus i alpha e raised to i k a plus b times b minus beta e raised to beta a plus b times c, minus minus plus beta e raised to minus beta a plus b times d equals 0, this is my question number 4. I am not going to reproduce this equation, but what I will right on the next page is that what I have the found the equation is some coefficient times a plus some coefficient times b plus some coefficient times d C plus some coefficient times d equals 0.

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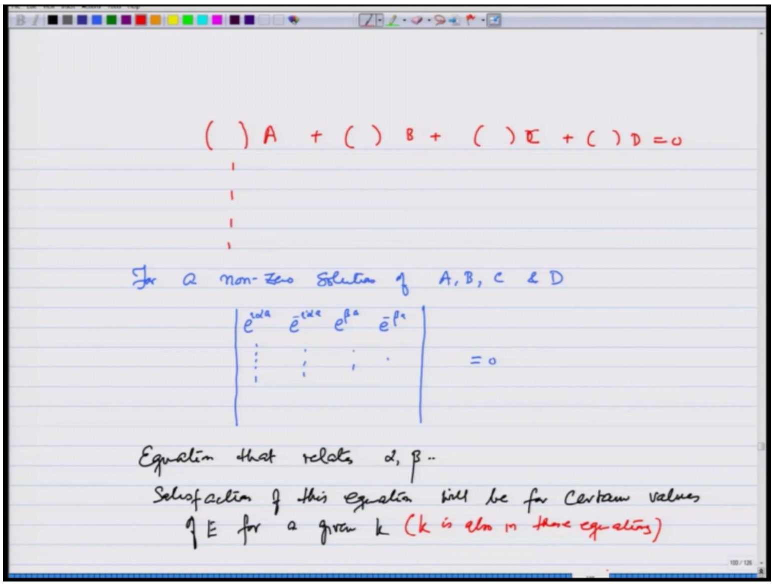

And I have 4 equations like this for a non-zero solution of A B C and D what should happen?

Now, because right hand side is 0 these are the determinant of these coefficients should be 0, determinant is whatever we wrote earlier e raised to i alpha a e raised to minus i alpha a e raised to beta a e raised to minus beta a and all those coefficients. So, you are in equation when you put this determinant you are in equation that relates alpha, beta and so on. And satisfaction of this equation will be for certain values of e for a given k where a given k, where does the k come from? It is also in these equations.

So, what you get is that you have this equation which involves alpha, beta, k, a function is equal to 0. So, you ask to computer now you scan over values of e for a given k, right? So, again I will restrict myself because I can do so by Bloch's theorem to k between minus pi by a and pi by a and ask the computer satisfy this function to be equal to 0 for different values of e for a given cases. So, suppose I do it for k equals 0 I will get some value here, one value here, one value here, one value here one value here, I do it for another k nearby either a value here.

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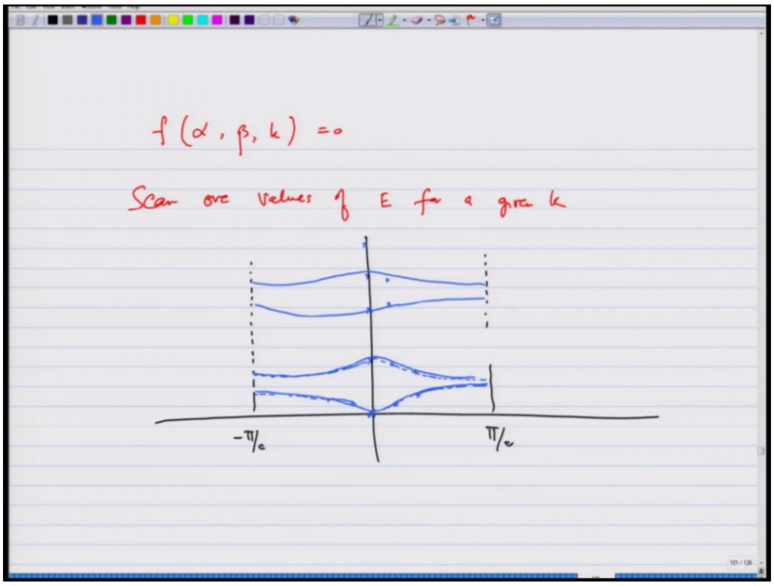

And you get a value here, I will get a value here, I get a value here and so on. Do it for the next k I will get another value here another value here I just do it for 2 bands I can do symmetrically for the other side.

And finally, when I join these points I am going to get a curve like this which is nothing but the energy band for each k there are several energies, but they form bands they continuously changing for each k because k is continuous and you get these bands. This is how the bands arise.

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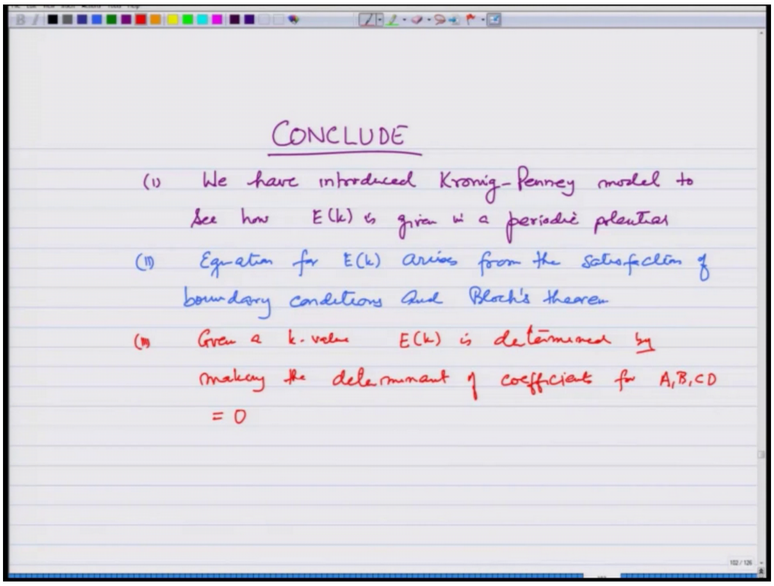

We see it more clearly in the next lecture when I do a simplified version of this Kronig-Penney Model. So, to conclude this lecture we have introduced Kronig-Penney Model.

So, to conclude this lecture we have introduced Kronig-Penney Model to see how e k is given in a periodic potential, right? Equation for e k arises from the satisfaction of boundary conditions and Bloch's theorem. Number 3 given a k value e k is determined by making the determinant of coefficients for and for the lack of better word I will just write A B C D equal to 0.

In the next lecture I am going to do a simplified version of this and show how these bands should necessarily arise.