Introduction to Solid State Physics
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Lecture - 63
Kronig- Penney model

So, far I have talked about Bloch's theorem, bands arising and also explained a bit about how band theory explains metals, insulators and semiconductors.

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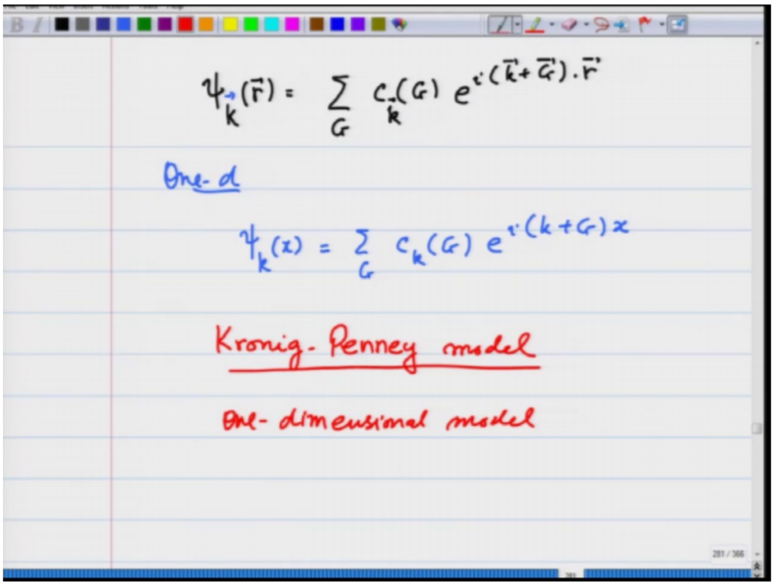

While getting the bands, what I had done was I had expanded psi k r as summation G c G for k th we have e raise to i k plus G dot r. This showed both Bloch's theorem as well as we used it for getting the bands and you have done it in your assignment also. We did other calculations in one d where psi k x was expanded I should write a vector here a summation G c k G e raise to i k plus G x where G was the reciprocal space vector and through this then we showed the one d Bloch's theorem as well as we got the bands also. In the assignment the problem that you have done is by mixing 3 plane waves.

In this lecture I want to solve an exact model again to show you the bands arising through Bloch's theorem. So, what I am going to do in this lecture is solve the Kronig-Penney model which is a one-dimensional model that shows how bands arise. So, we are looking at the band picture from another point of view.

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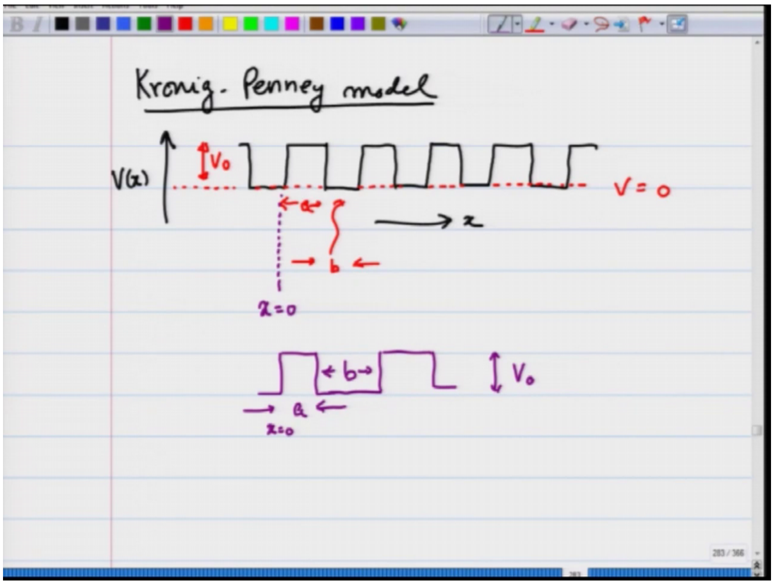

So, in the Kronig- Penney model we take a one dimensional potential which is of this form it is square well and barriers extending from minus infinity to plus infinity, what I am plotting here is along x direction I am plotting the potential V x. We can take this line red line that I am drawing red dashed line to be V equals 0. The height of the barriers to be V 0 and the width to be a for the barrier and b for the well and we want to solve for the energy Eigen value and the wave function in nutshell I want to solve the Schrodinger equation for this.

So, let me take this point to be x equals 0, so let me make the potential again from x equals 0 onwards. So, I have at x equals 0 extending from 0 to a. The potential barrier and then from a to b. The potential well and the height of the potential is V 0. So, I want to show you how Bloch's theorem is used to solve the Schrodinger equation in this particular case then we will simplify the model and solve it.

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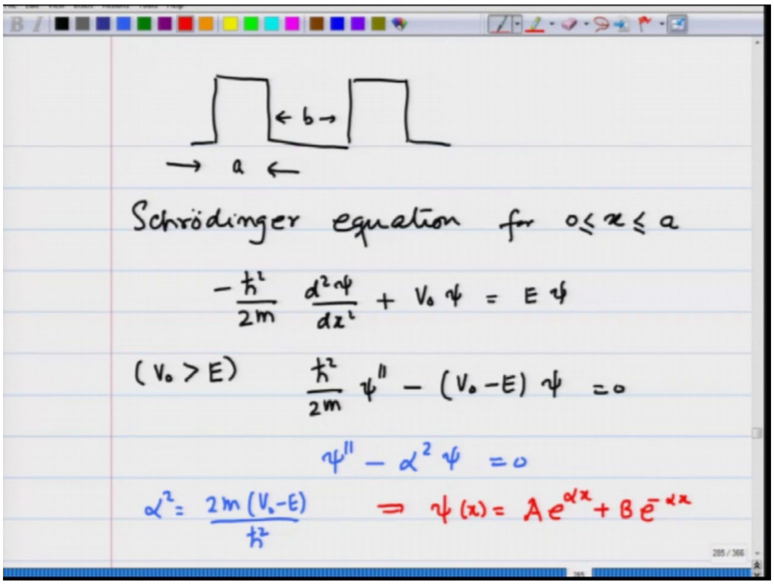

So, when I look at this potential extending form x equals 0 further down, so this is difference a and this is b. The Schrodinger equation for x between 0 and a is going to be minus h cross square over 2 m d 2 psi over d x square plus V naught psi equals e psi. I will assume V naught to be greater than e and then I have h cross square over 2 m psi double prime minus V 0 minus E psi equals 0. That is the equation and I can transform this equation into psi double prime minus alpha square psi equals 0.

Where alpha square is 2 m V 0 minus E over h cross square notice that I have taken V 0 to be greater than E, therefore alpha square is a positive number and this gives me solutions psi x equals A e raise to alpha x plus B e raise to minus alpha x. So, I obtain the solution in the region between 0 and a.

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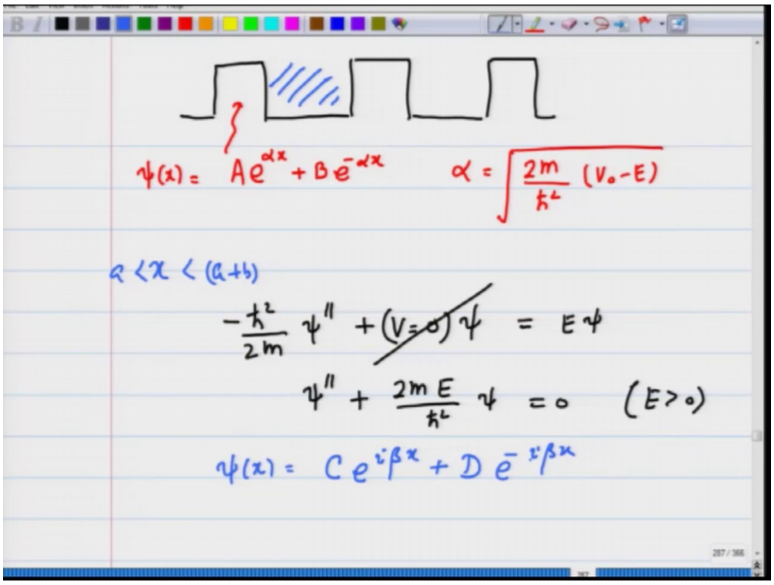

So let me make this potential again. And in this region I have got psi x equals A e raise to alpha x plus B e raise to minus alpha x, where alpha is equal to 2 m over h cross square V naught minus E square root. Now for the region x greater than a and less than a plus b, that is in this region which I am showing by blue shaded lines. In this region the Schrodinger equation is minus h cross square over 2 m psi double prime plus V is equal to 0 psi, so this term does not exist is equal to E psi. So, I get psi double prime plus 2 m E over h cross square psi equals 0. Keep in mind that E is greater than 0, because lowest potential energy is 0 and therefore I get solution for this region psi x equals C e raise to I beta x plus D e raise to minus I beta x. That is the solution in the second region.

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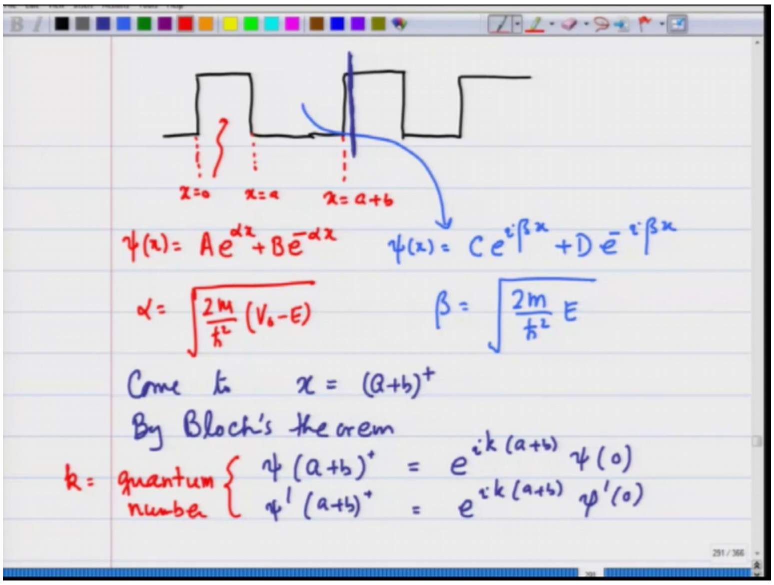

Let me show it again that when I take this potential in this region between x equals 0, x equals a and this is x equals a plus b, here on the left the wave function psi x is equal to A e raise to alpha x plus B e raise to minus alpha x. In the region next to it I have psi x equals C e raise to I beta x plus D e raise to minus I beta x, where alpha is equal to square root of 2 m over h cross square V naught minus E and beta is equal to 2 m over h cross square E square root, so far no Bloch's theorem has been used.

Now, you will see how Bloch's theorem determines the energy. If I come to x equals a plus b plus that is a point slightly outside x equals a plus b let me show this by this vertical line on the figure right here , right slightly to the right of x equals a plus b. Then by Bloch's theorem I would have psi at x equals a plus b plus is equal to e raise to i k a plus b psi at 0 and similarly psi prime at a plus b plus would be equal to e raise to i k a plus b psi prime at 0hat is using the Bloch's theorem and k is my is the quantum number that specifies the state psi k.

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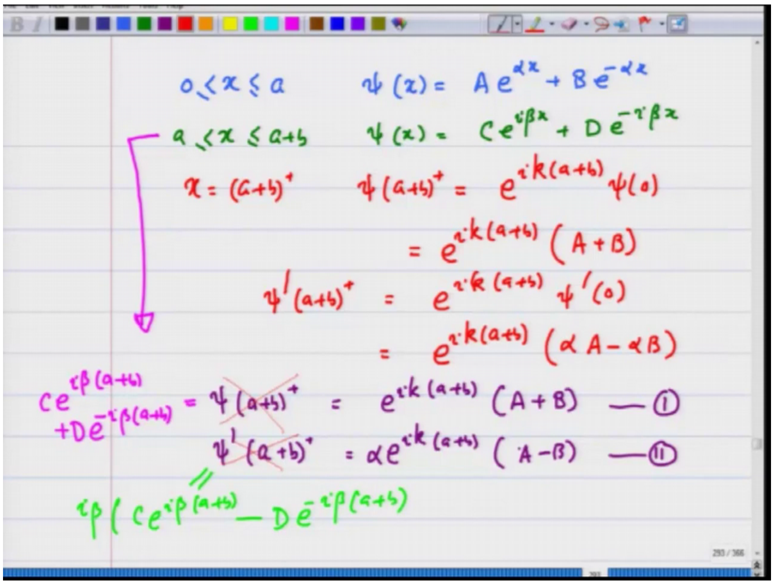

So, I have in the region x greater than 0 less than a, I have wave function psi x equals A e raise to alpha x plus B e raise to minus alpha x in the region x less than equal to a plus b greater than a. I have psi x equals C e raise to i beta x plus D e raise to minus i beta x and at x equals a plus b plus slightly to the right of a plus b, I have psi a plus b plus is equal to e raise to i k a plus b psi at 0 and this will be equal to e raise to i k a plus b and psi 0 from the first equation is nothing but A plus B and I also have psi prime a plus b plus is equal to e raise to i k a plus b psi prime at 0 and this will be e raise to i k a plus b alpha A minus alpha B.

So, 2 equations that I get from here are that psi a plus b plus is equal to e raise to i k a plus b a capital A plus capital B equation 1 and then I have I prime a plus b plus is equal to e raise to i k a plus b alpha A minus B equation 2. On the other hand psi a plus b should be same as psi at a plus b and that is calculated from this equation here and therefore psi a plus b plus is also equal to C e raise to i beta a plus b plus D e raise to minus i beta a plus b.

And similarly psi prime a plus b should also be equal to psi prime at a plus b calculate from the left hand side and therefore I am going to have i beta C e raise to i beta a plus b minus D e raise to minus i beta a plus b. So, these are 2 equations I can remove the middle part now, so let me do that I can just remove this part and these are the 2 equations relating C and D to A and B. I need 2 more equations on those 2 equations come from continuity at x equals a.

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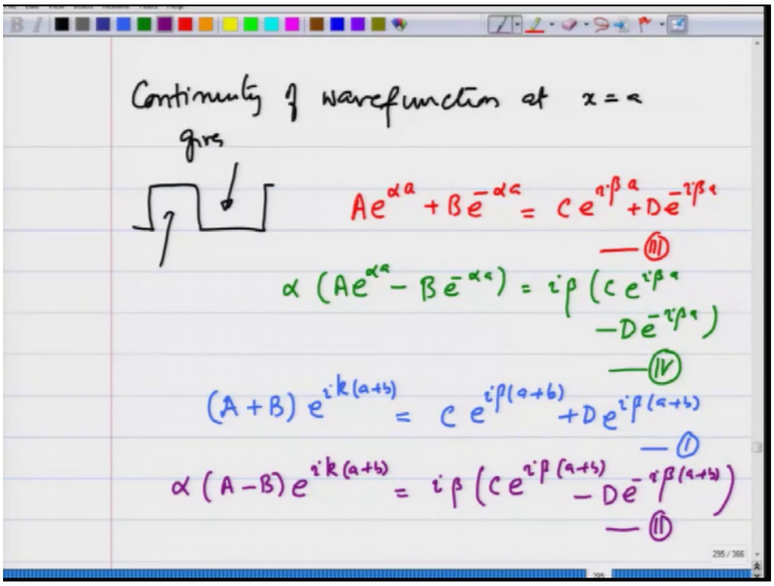

So, continuity of wave function at x equals a gives remember these are the regions I know wave function here I know wave function here. So, I am going to have A e raise to alpha a plus B e raise to minus alpha a is equal to C e raise to i beta a plus D e raise to minus i beta a that is my equation number 3 and the continuity of the derivative of the wave function gives alpha A e raise to alpha a minus B e raise to minus alpha a is equal to i beta C e raise to i beta a minus D e raise to minus i beta a. This is my equation number 4.

So, I have gotten 4 equations. I have written number 3 and 4 here number, 1 and 2 on the previous slide, but let me write them again here for completeness. So, number 1 and 2 were A plus B e raise to i k a plus b were equal to C e raise to i beta a plus b plus D e raise to i beta a plus b and this was equation number 1 and the second equation was alpha A minus B e raise to i k a plus b was equal to i beta C e raise to i beta a plus b minus D e raise to minus i beta a plus b this is equation number 2.

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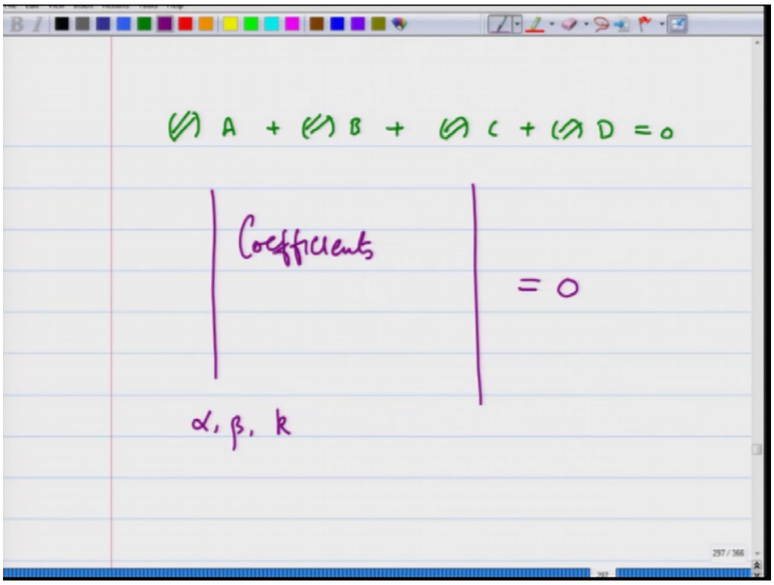

I have got 4 unknowns, 4 equations and I can put them in this form. Some coefficient A plus some coefficient B plus some coefficient C plus some coefficient D is equal to 0 like this there are 4 equations. So, I have these 4 equations and all of them go to 0 if A and B and C and D have to be nonzero, non trivial solution I should have this determinant of the coefficients is equal to 0 and that gives a relationship between alpha beta and k and through that I remember alpha and beta are related to energy and V 0, so through this I get e as E function of k.

I will now simplify all this part you should work out and I will give this as an assignment. I will simplify all this for the purposes of illustration here and reduce the number of variables due to by taking a very special form of Kronig- Penney model and in that what I will do is I will shrink the barriers to zero size and take these functions as delta functions.

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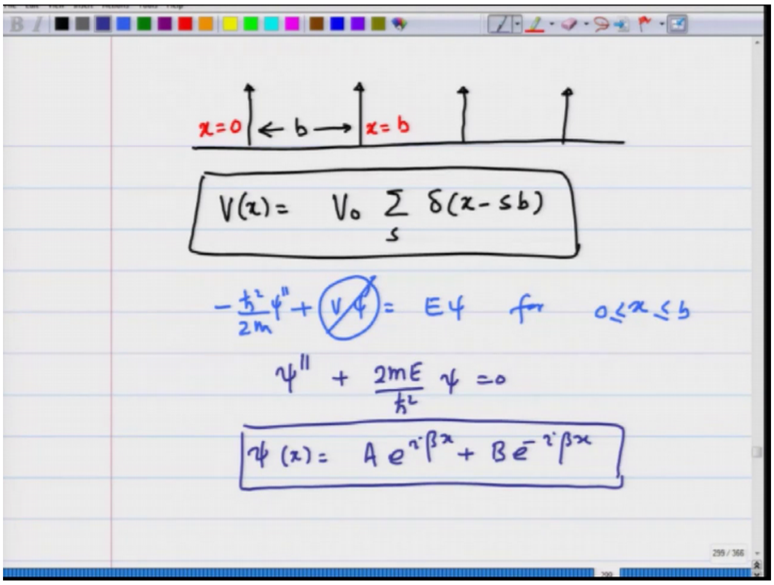

So, all these potentials V x, so I will take the potential V x to be of the form V 0 summation s delta x minus s b, where b is the distance between these barriers. So, I have shrunk the width a of the potential barrier to be 0 and increase the height to V 0. So, this is the potential which is periodic potential and here you will see that the number of variables are only 2.

So, again let me take the point at the first barrier to be x equals 0 and the other point becomes x equals b. If I take the solution of the Schrodinger equation E psi for x between 0 and b potential is 0 and therefore I get psi double prime plus 2 m E over h cross square psi equal 0 and I get psi x equals A e raise to i beta x plus B e raise to minus i beta x. That is the solution for the region between 0 and b.

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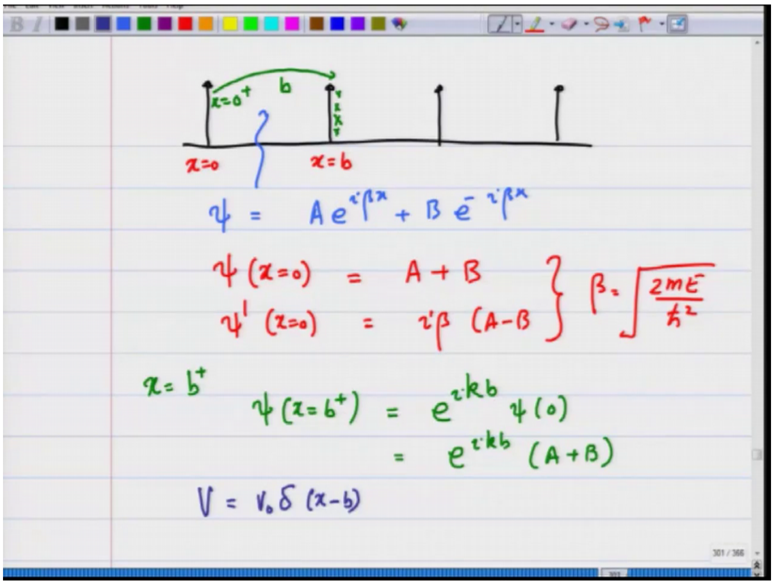

So, let me make this potential again. In this region I have got the solution psi equals A e raise to i beta x plus B e raise to minus i beta x. Point at the left barrier is x equals 0 and point on the right barrier x equals b. So, psi at x equals 0 is A plus B psi prime at x equals 0 is i beta A minus B. In both these beta is equal to square root of 2 m E over h cross square.

Notice that I have naught used Bloch's theorem so far which I am going to do now. Let us look at the point x equals b plus. That means, I am looking at a point here slightly to the right of x equals b and this point is displaced from x equals 0 plus y b. So, I can write that wave function psi at x equal's b plus by Bloch's theorem is going to be e raise to i k b psi at 0. So, this is going to be e raise to i k b a plus b. Now psi prime here is slightly settle.

Because I have a delta function between b plus and b minus. So, the potential at point b is delta V 0 delta x minus b and this gives a slight subtlety 2 the derivative of the wave function is not continuous and let us check that.

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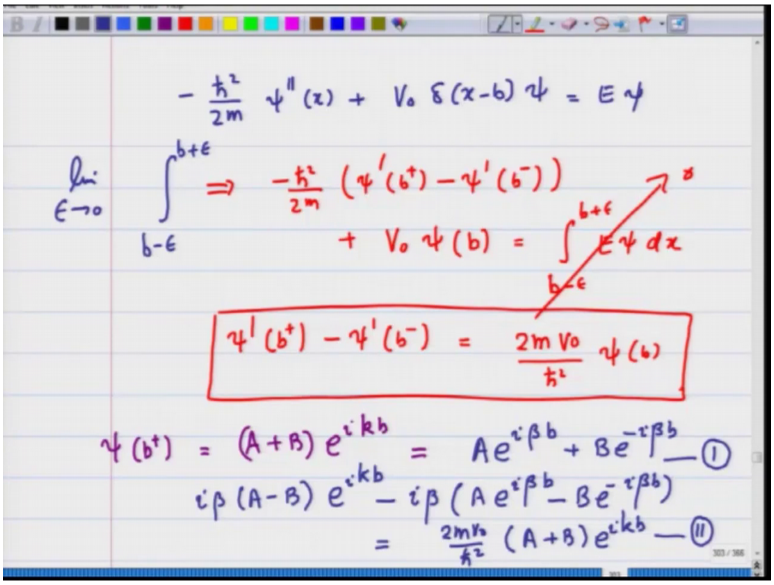

So, I have minus h cross square over 2 m, psi double prime x plus V 0 delta x minus b psi equals E psi. Let us integrate this equation form b minus epsilon to b plus epsilon where epsilon is tending to 0. When I integrate this I am going to get minus h cross square over 2 m psi prime at b plus minus psi prime at b minus plus V 0 psi at b. Keep in mind that the wave function psi is continuous, so at b plus b minus is the same is equal to e is finite. So, when I integrate form b minus epsilon to b plus epsilon E psi E psi being E and psi both being finite this fellow 0 and therefore I get psi prime b plus minus psi prime b minus is equal to 2 m V 0 over h cross square psi at b.

That is the condition on the derivative of the wave function. So, what we have found is 2 equations that relate the wave function across b and we have 2 unknowns a capital A and capital B, so that is all that is needed to solve the equation right. So, let us write this so I have the equation that A plus B e raise to i k b is the wave function at psi b plus and it should be continuous. Therefore this whole thing should be equal to the wave function coming from the left and that is A e raise to i beta b plus B e raise to minus i beta b. That is my equation number 1.

And equation number 2 gives the difference between the derivatives and therefore I get psi prime at b plus 1 is nothing but i beta A minus B and if I multiply by this by e raise to i k b this gives me psi prime at b plus 1 by Bloch's theorem minus psi prime at b minus and that will be i beta A e raise to i beta b minus B e raise to minus i beta b and this should be equal to 2 m V 0 over h cross square psi at b, which I can write either as A plus B e raise to i k b or A e raise to i beta b plus B e raise to i minus i beta b. I choose the former and this becomes A plus B e raise to i k b. This is my equation number 2. I have 2 equations, 2 coefficients A and B if I want a and b to be non trivial the coefficients of A and B must form a determinant that is 0.

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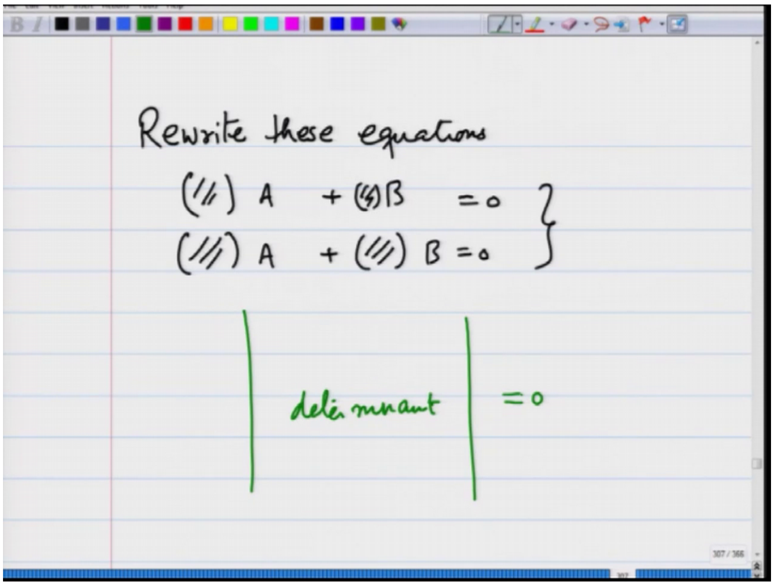

So, I do that so, I rewrite these equations as coefficient A plus some coefficient B is equal to 0 another coefficient A plus another coefficient B is equal to . These are my 2 equations which I have rewritten and then I write the determinant of these coefficients and make it equal to 0 and that leads to the equation and I am going to write the equation directly rest I will leave for you to work out and these equations when they are coefficients are made 0 they gave me m V 0 over beta h cross square sin of beta b plus cosine of beta b is equal to cosine of k b.

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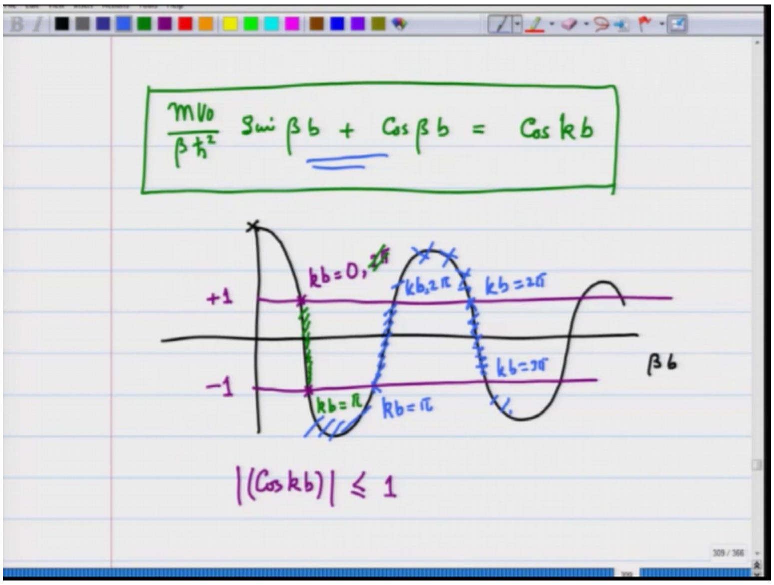

I will leave that working out to you. It is quite easy the only difference between the general Kronig- Penney that I obtained earlier and this is that right now my determinant becomes simplest 2 by 2 determinants and this equation I will now show you leads to band gaps. If I plot the left hand side, as a function of beta b, it starts at a high value and goes like this the value becomes smaller and smaller and this value out here is greater than 1. If I plot the limits plus one and minus one there like this, this is minus 1 this is plus 1. Now according to the equation written, the maximum value that this function can take is plus 1 and the minimum value it can take is minus 1 because cosine k b modulus is less than equal to 1.

So, when cosine k b is plus 1 I have k b equals either 0 or 2 pi and then you get energies continuously from here up to minus 1. So, k b equals pi so I will take k b equals 0 here. So 0 to k b equals pi you get continuous energy and at k b equals pi you see the energies where the value of the function on the left hand side here is greater than 1.This equation does not have a solution. So, at k b equals pi this point again is k b equals pi there is a gap in the energy, there is a gap in beta or beta times b that is there is no solution, this is the energy gap and again from k b equals pi to k b equals 2 pi, we have continuous energies. But as soon as you hit k b equals 2 pi again you go to a region where the equation is not satisfied and again k b equals 2 pi, so there is a gap and then again you have allowed solutions and then again k b equals 3 pi you have a gap.

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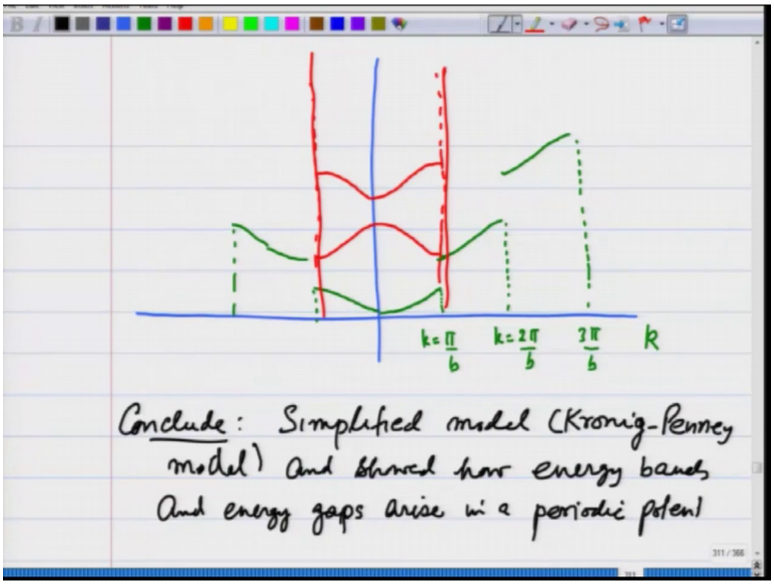

So, the situation is that if I were to plot the energy versus k you have up to k b equals pi some continuous energy this is k equals pi over b and then there is a gap, then again I have continuous energy up to k equals 2 pi by b and again there is a gap. Then I have continuous energy again up to 3 pi by b and then there is a gap. Same thing on the other side because the symmetry and then I can translate all these curves to the first Brillouin zone and make my second band like this and third band like this and so on, so in this zone I have this band structure.

So, what I have shown you through the simple Kronig- Penney model which was further simplified by taking the delta function barrier that by applying Bloch's theorem, we got energies which are continuous in the range 0 to pi by b for k and then at k b equals pi that is k times the periodicity length at each of these there is an energy gap that exists because the equation cannot be satisfied.

So, to conclude this lecture, we have taken a simplified model called Kronig- Penney model and showed how energy bands and energy gaps arise in a periodic potential.

Thank you.