Introduction to Quantum Mechanics
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Lecture - 04
Kroning-Penny model with periodic Dirac Delta function and energy bands

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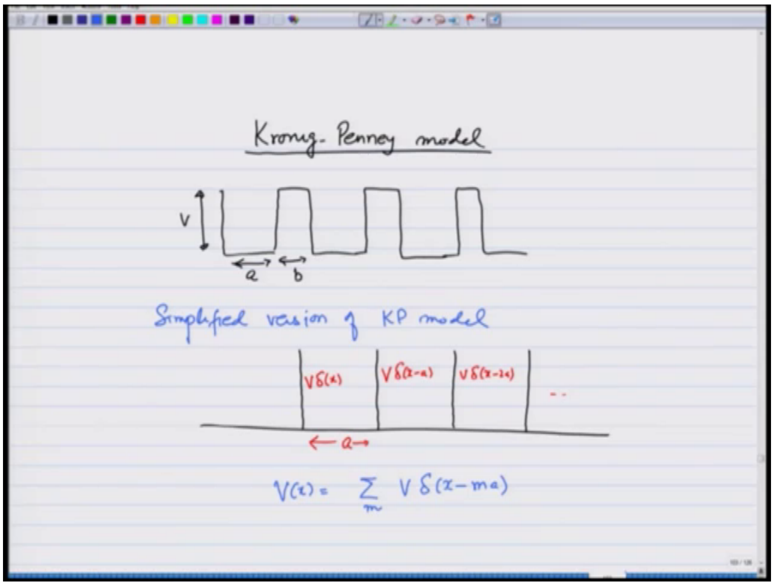

In the previous lecture I introduced the Kronig-Penny model where we had taken the potential to be the form shown here, where the height of the potential or some V and width of one portion of it was a and the other portion was b. And we derived an equation for the wave function and showed that if you take the determinant it gives you the energy versus k diagram.

Now, how those bands arise and why should there be bands can be seen in a simplified version of KP model which is also known as a Kronig-Penny model. And I am going to take an extreme in this and say that my potential actually consists of delta functions at each point. So, what we have done in a sense is taken these barriers to be of infinite height and made them of zero thickness and this distance is a and the potential is going to be given as delta x minus a here V delta x minus 2 a this is V delta x and so on.

So, the potential now is given as V x equals summation m V delta of x minus ma. And you can see this is periodic with period a. And we used to determine the energy versus k for this potential.

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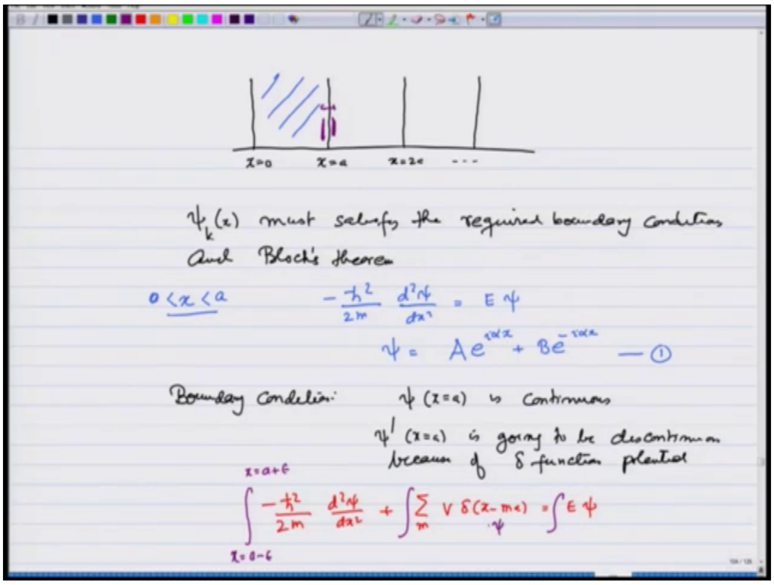

So, let me again make it. This is a potential, let us say this is at x equals 0 x equals a x equals 2 a and so on.

Again our strategy to determine the energy is going to be that psi k x must satisfy the required boundary conditions and Bloch's theorem; and that will lead to e k versus k picture. So, in the region x between 0 and a wave function is given by this equation minus h cross square over 2 m d 2 psi over dx square equals E psi because V is 0. And therefore, psi is nothing but an coefficient A e raise to i alpha x plus B e raise to minus i alpha x. So, in this region which is given like this.

Number one: now the boundary condition is like that for a delta function so it is going to be that; psi at x equals a is continuous and also psi prime at x equals a is going to be discontinuous in this case, because of delta function potential. And how much is the discontinuity let us do that. So, I have this Schrodinger's equation minus h cross square over 2 m d 2 psi over dx square plus at summation m V delta x minus m a equals E psi.

Let me integrate this from x equals a minus epsilon to x equals a plus epsilon. So, I am integrating just across this delta function I am showing it on the top of the screen, I am just integrating across the delta function I integrated everywhere; this is the psi here. So, what do I get?

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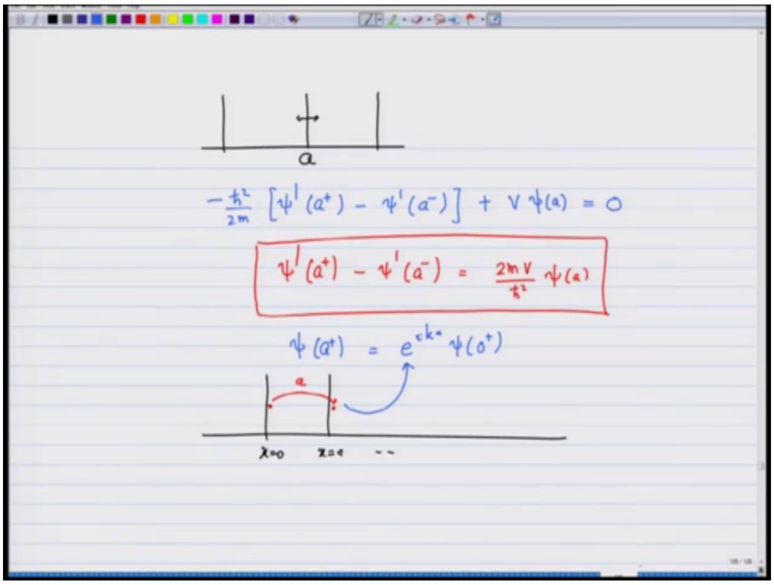

I get, let me show it again I am integrating across this delta function here at x equals a. So, I get minus h cross square over 2 m psi prime at a plus minus psi prime at a minus plus V psi at a is equal to 0. This we have done many times while doing the delta function potential, so I am not doing it in the details here I can always go back and check. And therefore, I get psi prime at a plus minus psi prime at a minus is equal to 2 m V over h cross square psi at a. That is my other equation of the boundary condition.

And I have psi at a plus is going to be equal to e raise to be I k a psi at 0 plus; let me show this through a picture again. So, I have this potential which is like this delta functions. I have the wave function let us say this is x equals 0, x equals a and so on. The wave function right here I will show it by red point. If I take the wave function on the other red point translate it by a the relationship is given, that is here.

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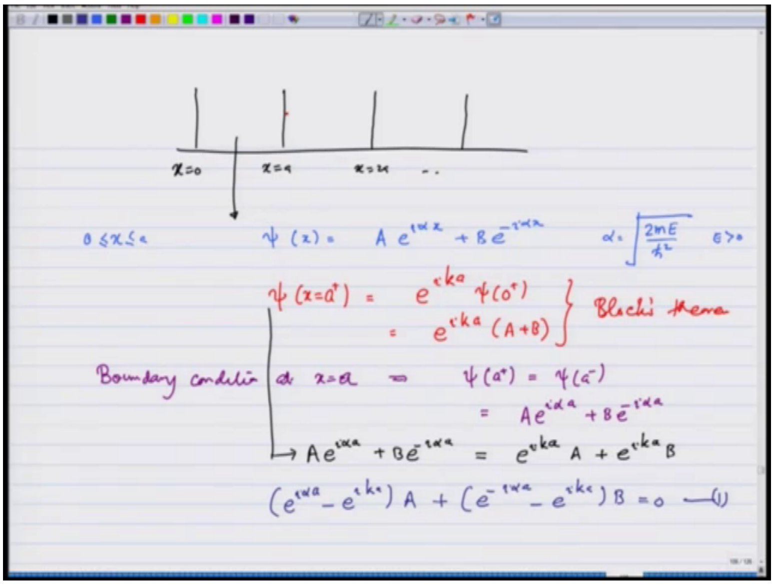

So, let us collect everything together. I have these combinations of delta functions x equals 0 x equals a x equals 2 a and so on, the wave equals this region between x o; x between 0 and a is given as psi x equals A e raise to i alpha x plus B e raise to minus i alpha x alpha being square root of 2 m E over h cross square. Notice that e is greater than 0. Then I have psi at x equals a plus just to the right of the delta function at a I will show it by this red spot is going to be equal to e raise to i k a psi at 0 plus which is nothing but e raise to i k a A plus B.

Now, since the wave function is continuous this is by Bloch's theorem, let me write that this is by Bloch's theorem. And boundary condition at x equals a tells me that psi at a plus is equal to psi at a minus and this is going to be A e raise to i alpha a plus B e raise to minus i alpha a.

And therefore, I have from the boundary condition and Bloch’s theorem together that A e raise to i alpha a plus B e raise to minus i alpha a which represents; let me make an arrow from here the psi at x a plus is equal to e raise to i k a A plus e raise to i k a B. And therefore, the equation that I have now for A and B is e raise to i alpha a minus e raise i k a A times a plus e raise to minus i alpha a minus e raise to minus i k a B is equal to 0 that is my equation number 1.

I still have one more equation to derive because there are two coefficients and that comes from the discontinuity of psi prime.

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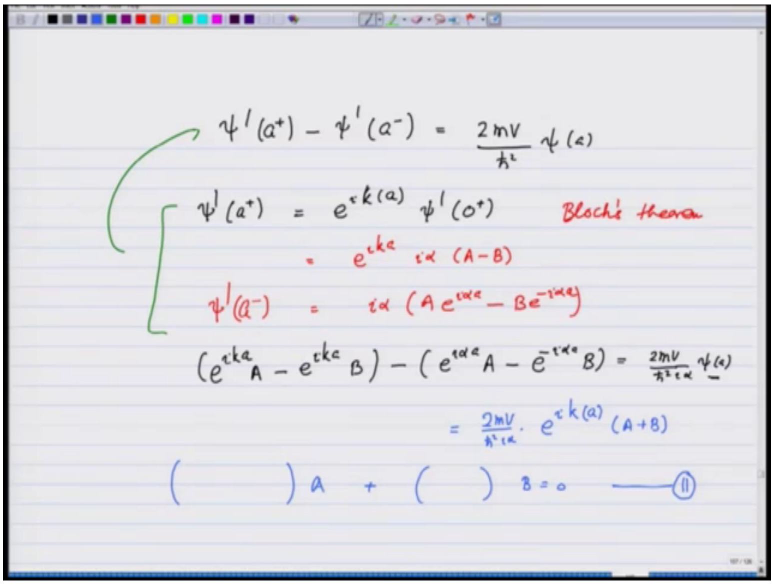

So, I have already said that psi prime a plus minus psi prime a minus it is going to be equal to 2 m V over h cross square psi at a. Now, a psi prime at a plus is going to be equal to e raise to i k a psi prime at 0 plus. This is by Bloch's theorem. So, this gives me e raise to i k a times I alpha a minus B. On the other hand psi prime at a minus is going to be equal to I alpha A e raise to i alpha a minus B e raise to minus i alpha a.

So, substituting these two in the equation here I get e raise to i k a A minus e raise to i k a B minus e raise to i alpha a A minus e raise to minus i alpha a B is equal to 2 m V over h cross square times I alpha psi at a. And psi at a we have already derived on the previous slide and that is nothing but is equal to 2 m V over h cross square i alpha. Psi at a plus and psi at a minus is the same, so I can write this as e raise to i k a A plus B.

Bring the terms from here to there and you get the second equation. With some coefficient here A, plus some coefficients here B equals 0 that is the second equation. I am not working out the details you can just work them out. Therefore, again I get two equations for A and B.

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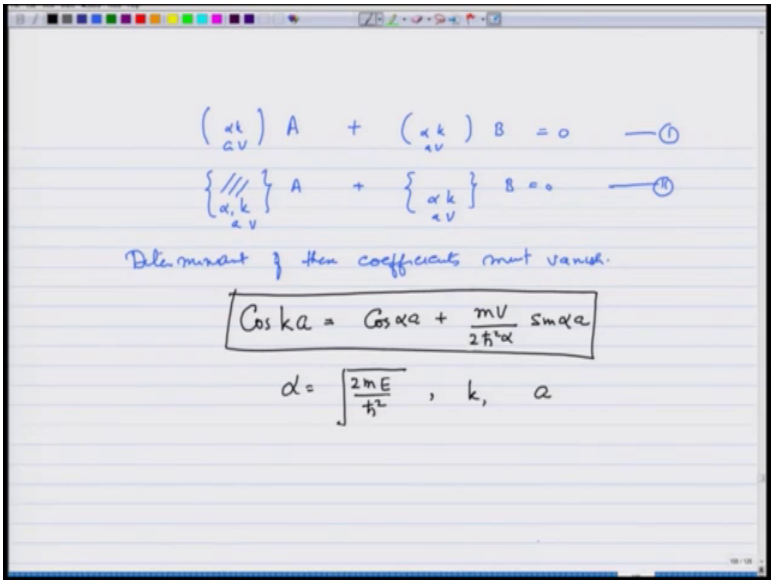

I have some coefficients times a plus some other coefficient times B is equal to 0; that is my equation 1. Some other coefficients times A plus some other coefficients times B is equal to 0; that is my equation 2. These coefficients are in terms of alpha k a V alpha k a V alpha k a and v.

And again for the solution to exist I should have that the determinant of these coefficients must vanish. I leave the writing that determinant and working this whole thing out for you. The final equation that we get after doing this and this is a simple determinants two-by-two matrix is cosine of k a is equal to cosine of alpha a plus m V over 2 h cross square alpha sin of alpha a; after you make the determinant 0.

Keep in mind that alpha is equal to square root of 2 m E over h cross square k some given k a is also given rest of the things are known. So, solution is given when equation satisfied.

Let us see; what does that lead to.

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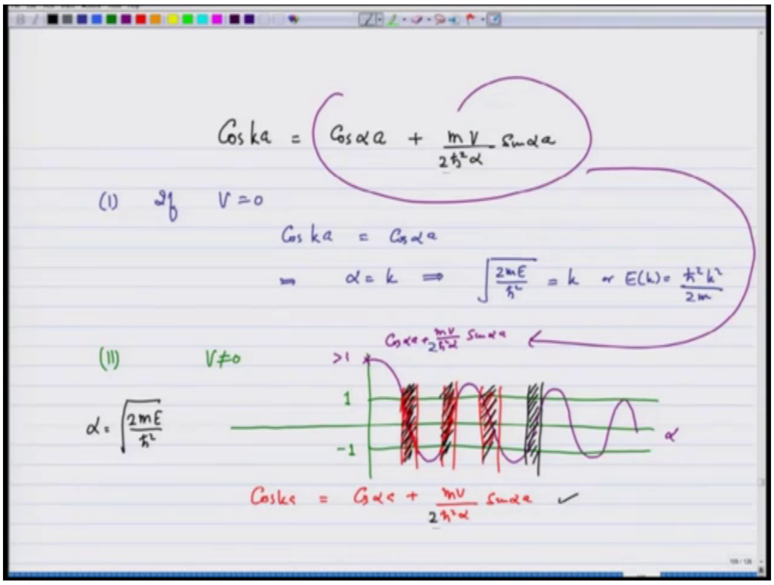

So, the equation I have is cosine of k a is equal to cosine of alpha a plus m V over 2 h cross square alpha sin of alpha a. Case one, if V is 0: if V is 0 is like free electron gas so what you want to have in that case is cosine k a is equal to cosine of alpha a. This means alpha is equal to k which implies square root of 2 m E over h cross square is equal to k or e k it is equal to h cross square k square over 2 m. That is the right answer.

What if V is not 0? Then the solution is given by wherever these equations is satisfied, but let us get an idea as to what solution would look like. So, if I were to plot alpha a versus the right hand side, so this is cosine of alpha a plus m V over 2 h cross square alpha sin of alpha a. Let us not keep it alpha a let us just keep it as alpha. So, if I were to plot right hand side this term versus alpha this would look like this. Amplitude will keep going down as alpha increases, because sin alpha is divided by alpha. This point is greater than 1.

On the other hand cosine k a maximum value is 1 and minimum value is minus 1; this is 1, this is minus 1. Since cosine of k a is equal to cos alpha a plus m V over 2 h cross square alpha sin alpha a, right hand side should not exceed one for solution to exist. So, solution would exist only in these regions. If alpha is between this point and this point solution exists.

So, let me make this read out here if alpha is between this and this point solution exists. If alpha is between this point and point solution exists. And for all the other region solution does not exists, now alpha is related to e. So, let me show it on the left hand side. Alpha is 2 m E over h cross square root. So, only if energy is in certain regions that I can find the solution for this equation, otherwise no. So, energy lies only in these bands. So, these bands arise from there.

So, what I have shown you is that if I take this extreme case of delta function potential it is very easy to see that bands arise solution exist, the Bloch's theorem and boundary conditions all are satisfied only for certain regions of energy, otherwise they are not. So, this tells you immediately why the bands exist.

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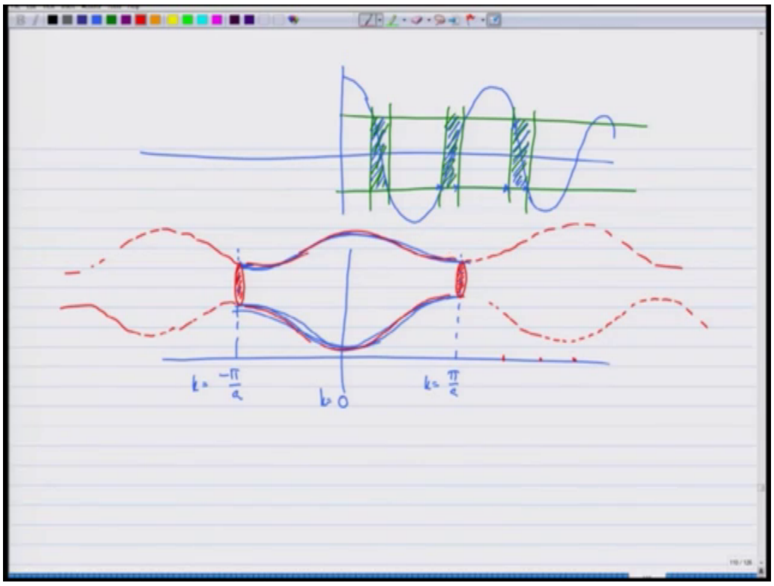

Now, if I have to plot is again and this is 1 and minus 1. So, only these regions give me energy that is allowed. And now if I have to plot energy versus k and that you can do by scanning over energy you will find that for a given k and again I can restrict myself to k between minus pi by a to pi by a you will get energy values like this, is perpendicular and so on.

And each of this band corresponds to the shredded region here. So, you can see for each man energy is either minimum or maximum depending on where this cuts this 1 and plus 1 and you will find that this is either k equals 0 or k equals pi by a or minus pi by a.

What our urge to do is look at this equation and try to plot these bands for different values of V and see what happens. You may also ask me question what happens if I take k larger after I can solve this equation for k larger. You will get energies which are like this, exact repetition of what is happening in the first (Refer Time: 20:08) zone. You will get energies which are like this; which again tells you that k actually you can restrict between the minus pi by a and pi by a and does not really matter, you get all the information about energies right here.

What is noticeable is that by introducing this delta function or periodic potential we have created a gap here which I am showing by this red ellipse and energy is lie in these bands. And this has implications which I will discuss a couple of lectures later.

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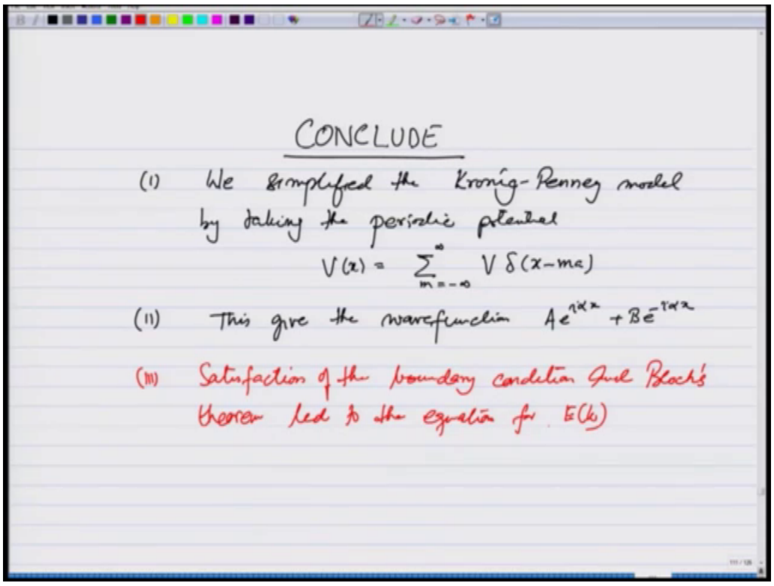

So, to conclude this lecture: one, we simplified the Kronig-Penny model by taking the periodic V x to be a combination of m equals minus infinity delta function potentials. And two, this give the wave function A e raise to i alpha x plus B e raise to minus i alpha x. And then three, satisfaction of the boundary condition and Bloch's theorem led to the equation for e k and that led to bands.