Physics of Nanoscale Devices
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Lecture - 06
KP Model

Hello everyone, as you might recall in our last class we started our discussion on the nature of electrons or the behaviour of electrons in solids. And we started discussing 1D solids and moreover 1D perfect solids in which there is no defect no lattice vibration.

And in that sequence of discussion we saw that we cannot solve Schrodinger equation precisely for the potential profile in solids and but there is an approximation which helps us a lot in order to solve the Schrodinger equation analytically and that approximation is known as the KP Model that we will discuss in today's class.

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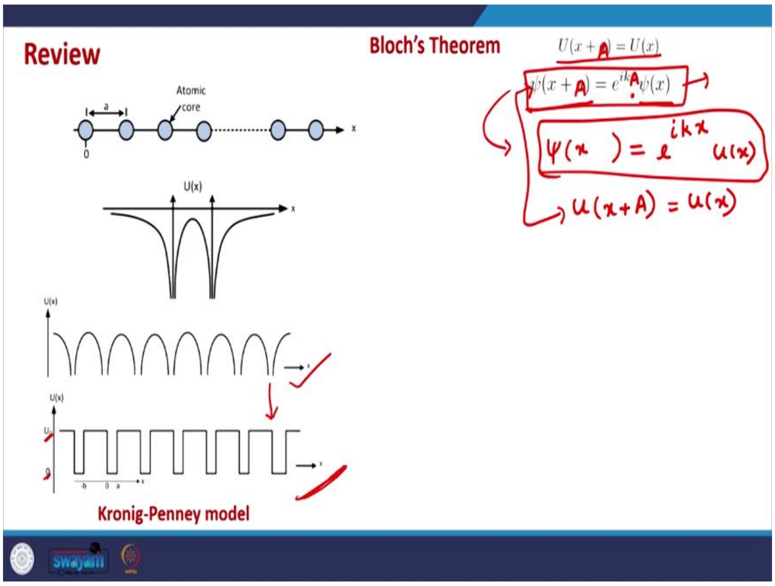

So, just to give a quick review a 1D solid looks a perfect 1D solid looks something like this it has a long sequence of atomic cores; atomic cores are positively charged, fixed and heavy particle so to say and in presence of these particles the potential profile the potential energy profile of the electrons will look like this. So, this is like an like a long sequence an infinite sequence of potential energy going to minus infinity and then going to an upper value and then again going to negative infinity.

But this is not an exactly solvable potential profile in Schrodinger equation. So, that is why the chronic penny model approximates this potential profile by a very similar looking profile, but we avoid the negative infinities in the potential profile and instead we have the potential going from a lower value which is taken to be 0 here to an upper value which is taken to be U naught periodically to the extent of the entire solid ok. So, this is what we discussed in last class.

This is what this is what we will solve the Schrodinger equation for, but even for this potential profile we cannot sort of solve the potential the Schrodinger equation for the entire extent of the solid because it is a it is like quasi infinite solid it is a very long solid in which if we had to solve the Schrodinger equation for the entire solid we would need to solve the Schrodinger equation for all the atomic cores corresponding to each atomic core.

But here as we saw in the last class a mathematical theorem called Bloch's theorem helps us and what Bloch's theorem says is that if the potential is periodic which means U(x+a) is equal to U(x) where U(x) is basically the potential profile. Then the wave function of the particle is given as $\Psi(x + A) = \Psi(x)e^{ikA}$ where A is the period of the potential profile potential energy ok.

And we also saw that an equivalence statement of this theorem is that this $\Psi(x + A)$ which means the wave function of the particle in this potential profile can be written as an equivalent statement is $\Psi(x)$ can be written as $\mathrm{u}(x)e^{ikA}$ where $\mathrm{u}(x)$ is a periodic function. Which means $\mathrm{u}(x + A)$ equals u(x) basically. So, we also saw that these two statements of Bloch's theorem are equivalent.

But what is the physical implication of Bloch's theorem? Physically it has made our job very simple because now we need to solve the Schrodinger equation in just one period of the potential profile and by using the Bloch's theorem either this statement or this statement we can find out the wave function of the electron or wave function of any particle anywhere in the solid ok. So, this is the power of the Bloch's theorem. This is highly useful theorem specially in a you know in solids or specially for potential profiles which repeat itself after certain distance ok.

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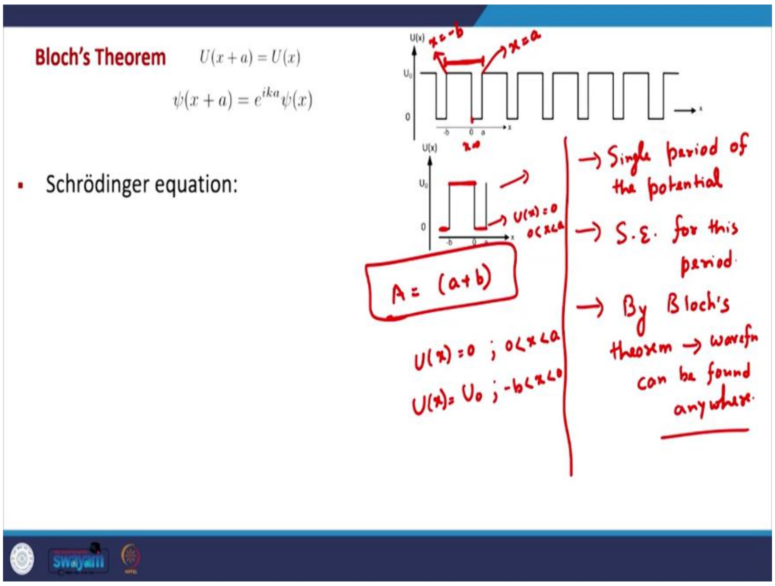

So, today we will see how the electronic wave function would look like in a 1D solid and for that we would first need to define a single period of the potential profile which means we would need to see how the potential energy looks like in a single period of itself because the potential profile is periodic and it repeats itself after certain time.

So, first we need to identify a single period or single length in which potential profile is not repeating itself and then we would need to solve the Schrodinger equation for this period ok. After that by invoking Bloch's theorem, By using Bloch's theorem we would be able to find out the electronic wave function everywhere the wave function can be find out anywhere in the solid ok. So, in this particular potential profile if we closely look at this we see that in this particular range of x values from here to here.

From this point to this point, this boundary to this boundary there is a single one iteration of the potential energy and after this the potential profile repeats itself with the same frequency basically ok. So, just for the sake of convenience we define this point to be the x=0 point we define this point to be x = a and this point to be x = -b. So, in this case the potential is having a certain pattern from x equal to -b to x equal to a ok and there is a jump in potential at x equal to 0 which is visible in this figure.

And then this particular pattern from x = -b to x = a it repeats itself throughout the entire solid. So, in this case the period of the period of the potential profile would be just a plus b. So, the potential repeats itself after (a+b) distance in space in this particular 1D solid.

So, with this background we are now ready to sort of solve the Schrodinger equation. So, the potential in this single unit cell for potential profile looks like this minus b to a and then it repeats itself.

And as we have seen a repeating potential or a periodic potential for a periodic potential we just need to solve the wave function for a single period and later on we can extend this wave function to the entire solid by using the Bloch's theorem. So, in this case in the in a single period of potential as visible from this figure there are two regimes of potential from x =0 to x =a the potential energy of the electron is 0 from x equal to 0 to a.

And the potential energy of the electron between -b and 0 is U_o . So, U(x) is 0 for x greater than 0 less than a between 0 and a and U(x) is a constant U_o between minus b and 0 ok and since the potential energy is different in these two regimes we would need to solve Schrodinger equation differently in these two different regimes ok. So, that is what we will do now we will solve the Schrodinger equation in these two regimes ok.

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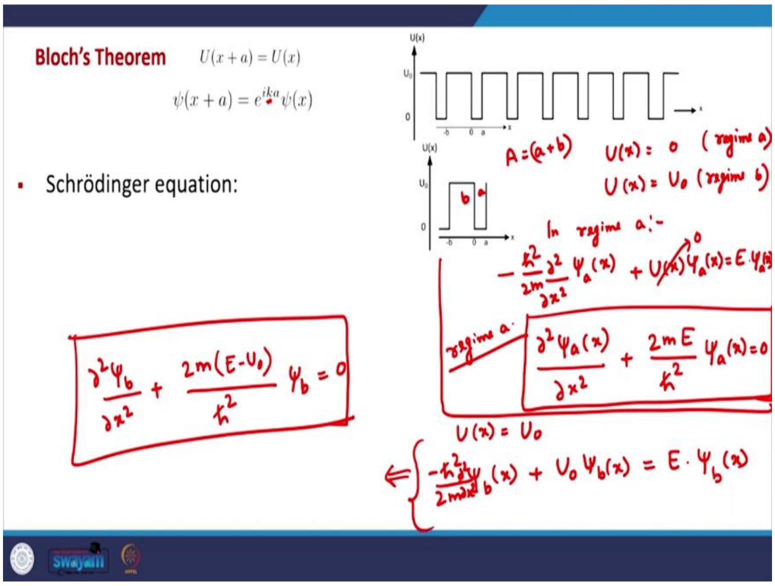

So, let us say this is regime a, this is regime b and as is clear the period of the potential profile is a plus b. I would take a pause here and sort of bring it to your notice that here this k parameter it comes from the Bloch's theorem. In our earlier derivations this k parameter was coming from the derivation of the Schrodinger equation, but here it is coming differently.

And if you go through the derivation of Bloch's theorem in any textbook you will see this k is still like the wave number it still corresponds to the momentum of the electrons in the solids, but it is slightly different from all previous cases. Physically it is still the momentum parameter and in this case it is known as the crystal momentum we will see that later on. So, first we will solve the Schrodinger equation and in regime a the potential energy is 0 and regime b the potential energy is U_o. regime a and regime b ok.

So, in regime a the Schrodinger equation would look like $\frac{-\partial^2}{\partial x^2}$, let us say the wave function here is $\Psi_a(x)$ plus U(x) $\Psi_a(x)$ equals E times $\Psi_a(x)$ ok, but in this case in regime a U(x) is 0. So, it essentially is and there is $\frac{-\hbar^2}{2m}$ as well here before $\frac{\partial^2}{\partial x^2}$. So, it would look like $\frac{\partial^2}{\partial x^2}\Psi_a(x) + \frac{2mE}{\hbar^2}\Psi_a(x) = 0$. So, this is quite like the Schrodinger equation for a free particle.

So, this is the Schrodinger equation in regime a of the potential profile in regime b the potential energy is U_o. So, the Schrodinger equation now would look like minus $\frac{-\hbar^2}{2m}\Psi_b(x)$ + $U_o\Psi_b(x)$ the wave function in this regime is basically $\Psi_b(x)$ represented as $\Psi_b(x)$equals energy of the electrons $\Psi_b(x)$. After rearranging these terms we can see that this can be written as and there is a double derivative here.

This can be written as $\frac{\partial^2}{\partial x^2}\Psi_b(x) + \frac{2m(E-U_o)}{\hbar^2}\Psi_b(x) = 0$. So, this is the Schrodinger equation in regime b. So, let us sort of put them together at one place and as you might have already noticed the Schrodinger equation looks quite like our earlier Schrodinger equations that we solved for free particle and particle in a box cases.

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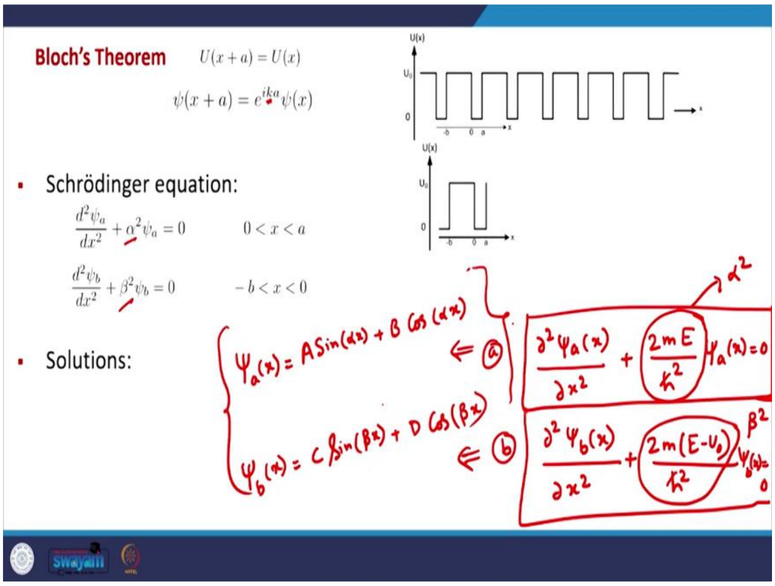

So, putting them together Schrodinger equation for regime b would be $\frac{\partial^2}{\partial x^2}\Psi_b(x)$ + $\frac{2m(E-\mathrm{U_o})}{\hbar^2}\Psi_b(x)$ = 0 ok. So, this is a regime a and this is regime b ok. So, this parameter can be defined as sort of alpha parameter α^2, let us define it to be alpha square and let us define this to be β^2 as is clear here.

So, once we define once we sort of encapsulate this energy term in alpha and beta then we can easily write down the solution of these Schrodinger equations in terms of sines and cosines as we did earlier in case of free particle and particle in a box. So, the solutions of the Schrodinger equation will look like this in regime a $\Psi_a(x)$ would be given as Asin(αx) + Bcos(αx) and in regime b $\Psi_b(x)$ can be written as Csin(βx) + Dcos(βx).

So, these two are the solutions of the Schrodinger equation in regime a and regime b respectively. As you can see there are four unknowns here and in order to solve in order to precisely find out the values of these unknowns we need to use boundary conditions as we did in case of particle in a box case ok.

So, please remember these solutions specially the free particle solution and particle in a box case because these two solutions are easy to remember first of all and second these two are heavily used prototypes solutions in almost all quantum mechanics specially in solid state physics ok. So, please keep those things in mind and now we need the boundary conditions for this particular system.

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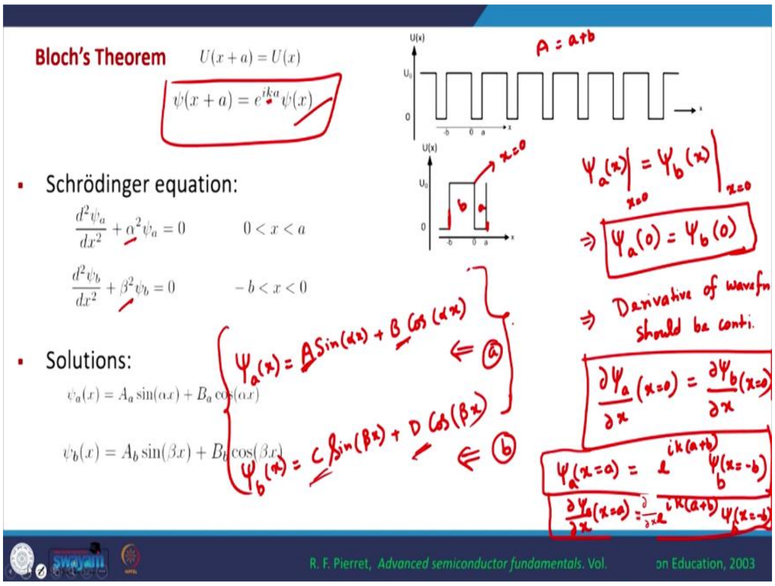

And so there is one boundary here at x equal to 0 ok. So, the boundary condition at x equal to 0 basically means that from the postulates of quantum mechanics you might have easily guessed that the first boundary condition would be that the wave function should be continuous at x equal to 0. What it means is that Ψ_a which is basically the wave function in regime a at x equal to 0 should be equal to Ψ_b which is the wave function in regime b should be equal to $\Psi_b(x)$ at x equal to 0.

So, the first boundary condition would be that $\Psi_a(0)$ should be equal to $\Psi_b(0)$ that comes from the continuity of the wave function as we discussed in the postulates of the quantum mechanics ok. So, this is the first boundary condition that we would use .The second boundary condition is that the derivative of the wave function should be wave function and should be continuous. Which means that derivative of $\Psi_a(x)$ at x =0 should be equal to derivative of $\Psi_b(x)$ at x =0.

So, these two boundary conditions we obtain from the basic postulates of quantum mechanics ok, but there are 4 variables and we need at least 4 conditions to solve for all 4 unknowns here these A, B, C and D. So, the other two boundary conditions will come from the Bloch's theorem itself and according to this theorem the potential as we can see in this single unit of potential profile the potential profile repeats itself after the interval of a plus b.

So, it means that the potential here and here are again same potential at x = -b is again same as potential at x =a. So, what it means is that $\Psi_a(x=a)$ is $\Psi_b(x=-b)e^{ik(a+b)}$. So, this comes from the Bloch's theorem from this statement of the Bloch's theorem and similarly a similar statement of Bloch's theorem holds true for the derivative of the wave function. And from there we can see that $\frac{d\Psi_a}{dx}(x=a) = \frac{d\Psi_b}{dx}(x=-b)e^{ik(a+b)}$. ok.

So, this Ψ(x=-b) is basically Ψ_b function and Ψ(x=a) is Ψ_a function similarly here and here. So, now, these are the 4 boundary conditions that we will use in order to find out these 4 unknowns A, B, C and D in the solution of the wave function ok.

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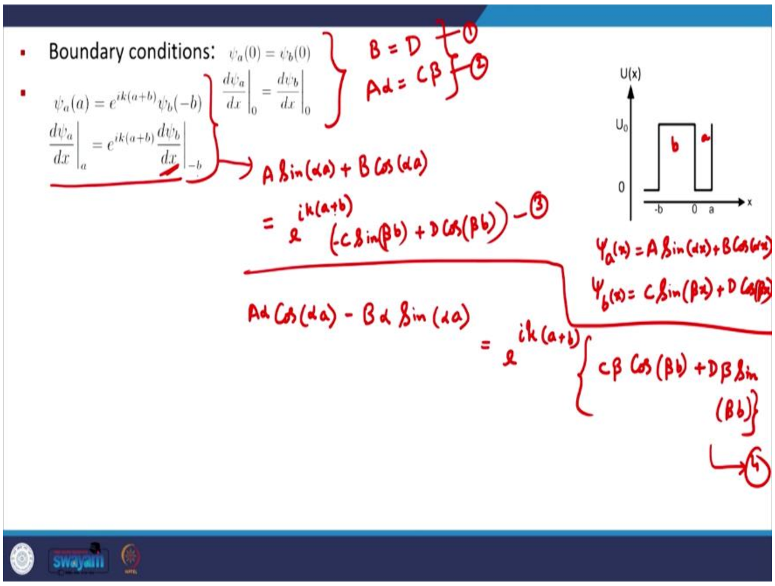

So, once we can find out these four sort of ,once we solve these four equations if we solve for. So, for example, if we solve the first equation first boundary condition. Now, things are getting the maths is getting slightly involved as we are progressing in real systems and that is the characteristics of quantum mechanics for most of the practical systems it is mathematically difficult.

So, in this if we use this boundary condition $\Psi_a(x=0)$. So, if we put x=0 in this case the first term would be 0 and the second term would be b times 1.

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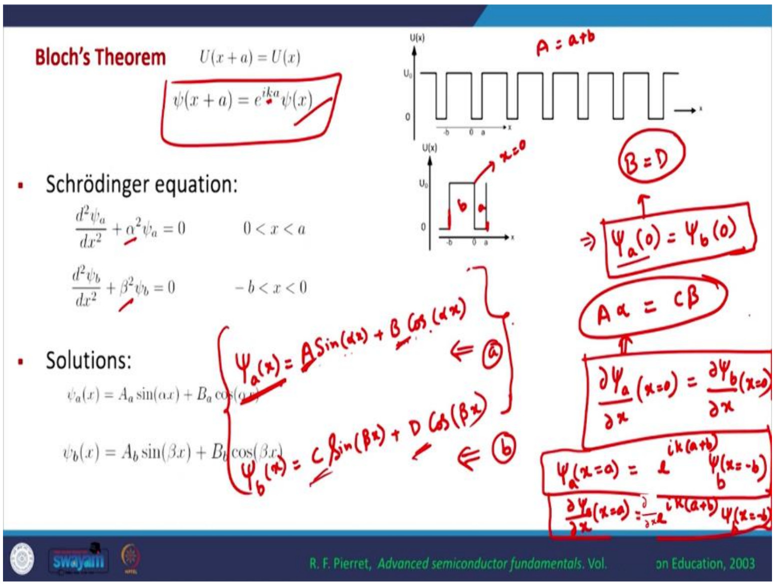

So, this boundary condition says that $\Psi_a(0)$ is B basically and $\Psi_b(0)$ is similarly D. So, this says that B should be equal to D and the second boundary condition says that if we take the derivative of the wave function $\Psi(x)$, $\Psi_a(x)$ it would be $A\alpha\cos(\alpha x) + B\alpha(-\sin(\alpha x))$ and at x =0 it would be A times α and similarly it would be C times β.

So, these are two conditions or two relations that we obtain from the boundary conditions. So, from the boundary condition from these two boundary conditions we can directly see that B should be equal to D and Aα is equal to Cβ. This is regime a this is regime b the wave function in regime A is $A\sin(\alpha x) + B\cos(\alpha x)$ and wave function in regime b is $C\sin(\beta x) + D\cos(\beta x)$ ok.

So, we have already obtained two constraints which will give us the values of these constants and the other two constraints can be obtained from the boundary conditions arising from the Bloch's theorem and if we use Ψ_a equals a Ψ_a at x=a it will be $A\sin(\alpha a) + B\cos(\alpha a)$ that should be equal to exponential.

So, this $A\sin(\alpha a) + B\cos(\alpha a)$ should be equal to $e^{ik(a+b)}\Psi_b$ at x=-b which is Ψ_b at x =-b would be $C\sin(-\beta b) + D\cos(\beta b)$. So, this is the third this is constraint number 1, this is constraint number 2, this is constraint number 3 and the fourth constraint will come from the derivative of these wave functions which is essentially.

So, if we take the derivative of Ψ_a with respect to x it will be $A\alpha\cos(\alpha x) - B\alpha\sin(\alpha x)$ and its value at a would be $A\alpha\cos(\alpha a) - B\alpha\sin(\alpha a)$ should be equal to e$e^{ik(a+b)}$ derivative of Ψ_b at x =-b. So, derivative of Ψ_b would be $C\beta\cos(\beta x) - D\beta\sin(\beta x)$ and at x=-b it would be $C\beta\cos(\beta b) - D\beta\sin(\beta b)$.

So, this is constraint number 4. So, we have 4 constraints 4 unknowns are there A, B, C and D in principle by using certain mathematical techniques we can solve these constraints and we can find out the values of A, B, C and D. So, we can easily sort of replace B by D in constraint number 3 and 4 and we can replace A by C times beta by alpha and by putting these values of B and A in equation 3 and 4 we will be left with only two constraints and these two constraints can be solved or will have a non trivial solution if the determinant of the coefficients of the unknowns in these constraints is 0.

So, this is a standard mathematical technique from matrix algebra that these two constraints will have non trivial solution when the determinant made from the coefficients of the unknowns will be of value 0 . So, finally, by putting the determinant of the coefficient to be equal to 0 this is what we finally, obtain.

$$\frac{1-2\xi}{2\sqrt{\xi(|1-\xi|)}}\sin(\alpha_0 a\sqrt{\xi})\sinh(\alpha_0 b\sqrt{|1-\xi|})+\cos(\alpha_0 a\sqrt{\xi})\cosh(\alpha_0 b\sqrt{|1-\xi|})=\cos(k(a+b))$$

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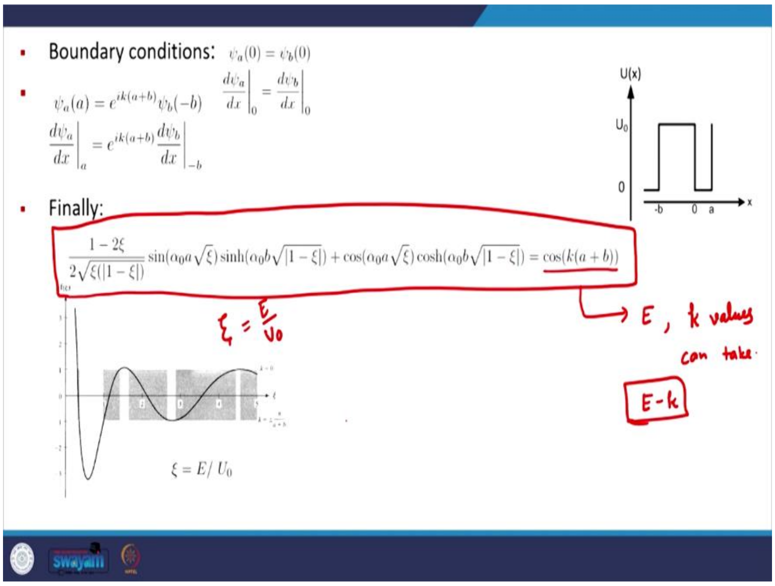

This is the final relationship that gives the valid solutions of the Schrodinger equation. On the left hand side we have this parameter which is essentially E/U_o on the right hand side the left hand side is a function of E as you can see and the right hand side is a function of k just, apart from these two things all other parameters are system parameters or constants.

So, there so in a way this equation basically tells us about the relationship between the energy of electrons that can exist in a solid and the k values that these electrons can take in the solids or in other words this is the E-k relationship for solids this constraint give us the E-k relationship between solids ok. Please remember I would again remind you that this k comes from the solution of the Bloch's theorem from the statement of the Bloch's theorem and this is known as the crystal momentum or the momentum of electrons in a certain environment.

And it is different from the k that we generally use in the solution, but physically mathematically it is coming from a different source, but even in Bloch's theorem it is coming from the solution of the Schrodinger equation. So, do not worry about that physically it corresponds to the to a parameter called crystal momentum ok and again a mathematical solution is not impossible it can be done, but a graphical solution would be easier to understand which is our aim in this particular course ok.

So, we will see how the solution of this equation looks like and that will give us the valid results in this particular solid. So, if we plot the left hand side and the right hand side of this equation on the same axis. we will get the solution and that is what we will see in the next class ok.

Thank you for your attention. see you in the next class.