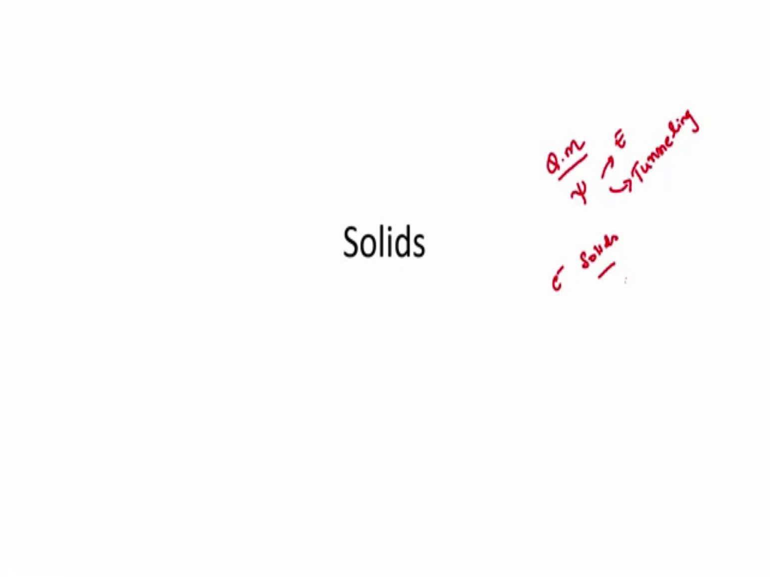
Semiconductor Devices and Circuits

Prof. Sanjiv Sambandan
Department of Instrumentation and Applied Physics
Indian Institute of Science, Bangalore

Lecture - 04
Solids: Formation of Bands, Kronig-Penny Model

(Refer Slide Time: 00:18)



Solids

Q.M

$\psi \rightarrow E$

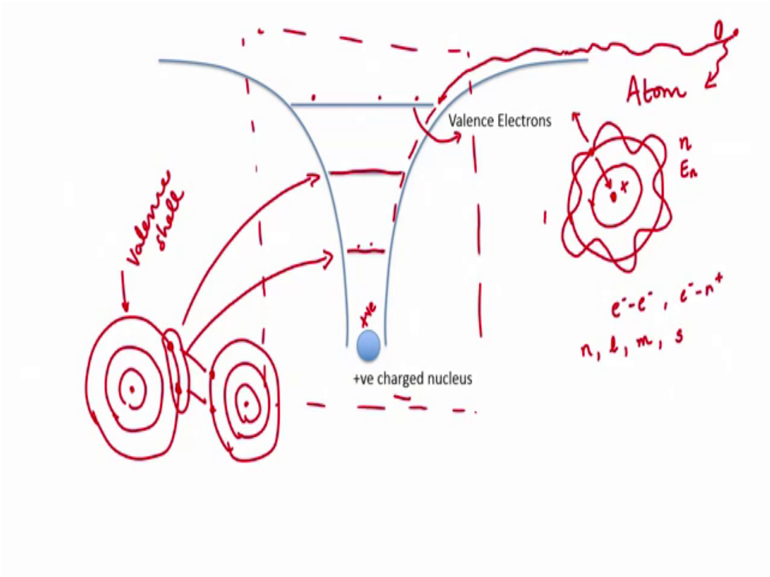
→ Tunneling

e Solids

So, far we have looked at quantum mechanics, which described the behaviour of the wave particle via, the wave functions psi. And it described the physics and the behaviour of very tiny particles such as electrons and said that there was some very interesting behaviour such as the quantization of energy, such as the aspect of tunnelling through a barrier etcetera, which could not be explained by classical mechanics.

We are now in a good position to start understanding the behaviour of electrons in solids. And over the next few lectures, we will describe, what happens we will describe the nature of electrons in an atom, and we will also describe the construction of a solid by bringing several atoms closer to each other, and how this actually influences the behaviour of electrons in a solid.

(Refer Slide Time: 01:17)



So, to start off let us just look at the atom. And we for an atom, we have a positively charged nucleus and you have an electron, we have electrons going around this nucleus, this positively charged nucleus. In fact, you have an electron cloud, because you only have a certain probability of finding the wave electron at any particular location.

And in order to study, the behaviour of the electron around the nucleus. In your high school you might have looked into several models, where in you would have equated the electrostatic forces of attraction, with the centrifugal forces, experienced by the electron. And also taken into account, the wave nature of the electron by placing a constraint that there should be an integer times, the wavelength present along each present around each orbit. And this result this would have resulted in a certain quantum number, which would have resulted in the quantization of energies.

Now, if we solve sorting this equation for an atom, the potential energy term will have to take into account electron, electron interactions in the atom, and the electron nuclear interactions in the atom. And by solving Schrodinger's equation, we find that for a 3-D atom, we will end up with several quantum numbers. And you might also be familiar with these quantum numbers from your high school, and you might have heard of quantum numbers such as the principle quantum number, the azimuthal quantum number, the magnetic quantum number, and the spin quantum number.

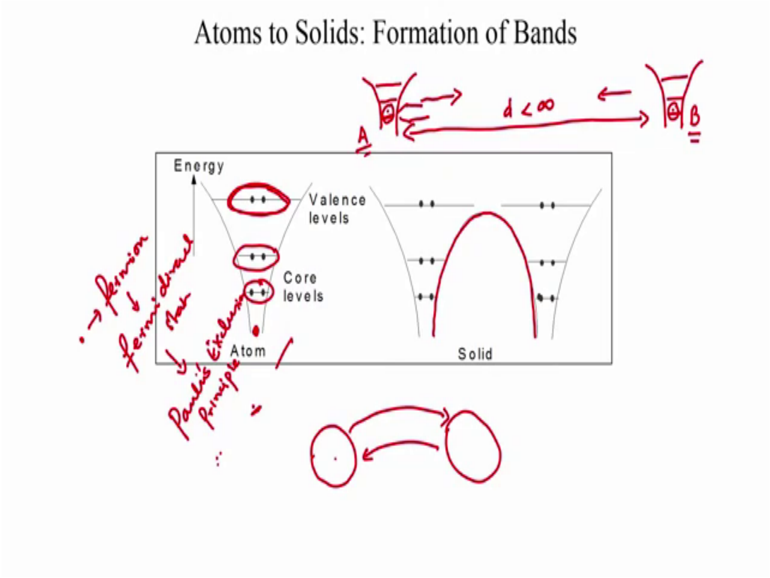
So, therefore, in an atom, we have, we have electrons occupying discrete energy levels inside the atom. So, what I have shown here is the potential profile for a positively charged nucleus, and in some sense this entity here represents the atom. So, if an electron were to be present say infinitely far away from the nucleus, it would not see any of this potential and we could say that the potential experienced by this electron is 0.

The electron would be at 0 potential and therefore, it would be completely free to move about, and absolutely free from any forces produced any forces prescribed by this positively charged nucleus. But as the at electron starts approaching this positively charged nucleus, it starts experiencing this potential well and it is drawn into this potential well and it eggs and it can experience many stable states inside deeper inside this well. So, therefore, these different shells of an atom.

In some sense relate to these energy levels as shown in this figure. So, here you have these different energy levels, and you have electrons occupying these energy levels, and the outermost shell is something called as the valence shell. And the electrons occupying the outermost shell are called as the valence electrons.

Now, these electrons are quite important, because they are the ones that decide or you know that participate in any interaction between two different atoms. So, if we have two atoms, it is the valence electrons of these atoms that participate in bonding or interact, and any interaction between these atoms. So, this is the picture of the electrons in an atom.

(Refer Slide Time: 05:19)



Atoms to Solids: Formation of Bands

Now, what happens when you start bringing several atoms closer to each other. So, here you have a single atom and you have all these electrons that are sitting closer to the nuclei, and are more tightly bound to the nuclei. Whereas, the valence electrons are the father ís I mean other, other farthest away from the nuclei and therefore, they experience the least amount of binding to the nuclei.

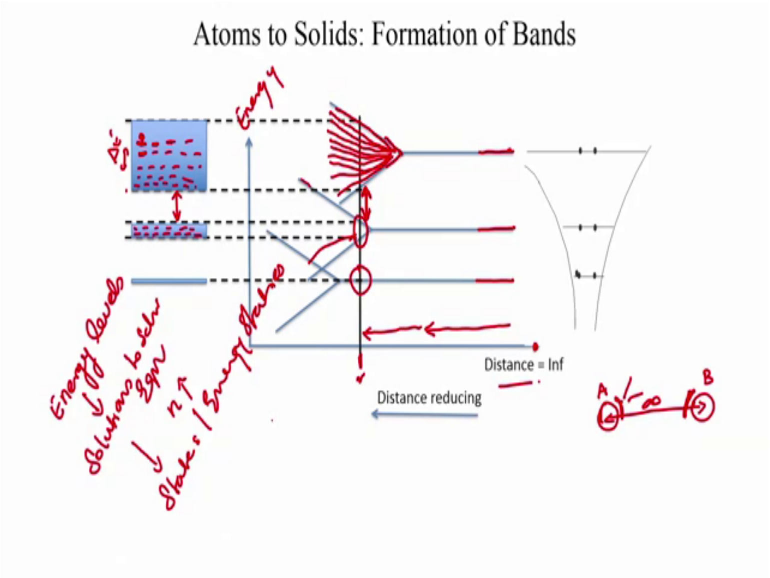
Now, when you start bringing two different atoms closer to each other the electrons in each of these atoms begin to interact, and what do we mean by that. So, let us take two atoms A and B ok. So, let us say we have atom A, and we have an exactly identical atom, which is called atom B ok. And let us say to start with these two atoms are infinitely far apart ok.

So, the distance between them is infinite, which implies that atom B has no knowledge of atom A it does not feel atom A at all; and atom A does not know anything about atom B. So, in these two atoms the electrons would occupy, the energy levels as prescribed by Schrodinger's equation, and in fact, both these atoms since they are both identical the electrons would be occupying very identical energy levels in each of these atoms. But the moment we start bringing these atoms closer to each other. So, we let us, let us now start reducing the distance between these atoms. So, the moment we start bringing these atoms closer to each other, we find that the electrons now begin to feel each other in the sense that the atoms now learn of each other's presence.

Now, electrons are fermions and they, they follow something called as a Fermi-Dirac statistics, which we will describe later in this course. And therefore, they have to obey something called as the Pauli's exclusion principle. And what Pauli's exclusion principle tells us is that it places a constraint ok. It says that note no two electrons can have all their quantum numbers the same, which is no two electrons can have can occupy the same exact same energy level or energy state. And, because of this limit, when we start bringing atoms closer to each other, we find that these electron energy levels have to start splitting ok, they need to they can both these energy levels cannot remain the same, and the energy levels start splitting in order to accommodate the extra electrons that are appearing, because of the two atoms.

So, this interaction between two atoms is in a simple manner described here, and we will describe it a little better in the next slide. But what you see here is here you had the first atom, which had it is own potential profile, and then we had the second atom which had it is own potential profile. And the moment we start bringing these two atoms closer to each other, these potentials these potential profiles begin to interact, and you start seeing a potential profile that looks like this.

(Refer Slide Time: 08:49)



Atoms to Solids: Formation of Bands

So, let us look at the splitting of energy levels a little better. So, I here have a very crude drawing, which shows this aspect. So, let us say the so what we have here is a plot of energy versus distance between the atoms. So, so this distance is the distance between the two atoms A and B that, we were talking about. So, initially this distance is infinite; so initially we start off at infinite. And we look at the energy levels of each of occupied by these electrons.

So, since the atoms are infinitely apart, the energy levels are very are identical, and there is absolutely no splitting in the energy levels, because the atoms do not feel each other. But as we start bringing the atoms closer to each other, the valence electrons or the valence shell first begins to respond the energy levels in the valence shell begin to start splitting, because they feel the other atom the earliest.

So, as we start reducing the distance between the atoms, these outermost electrons the energy levels here begin to split and as we bring them closer and close as it start bringing these atoms closer and closer, the inner shells also begin to feel, the presence of the other atom. And the energy levels and the inner shells will also begin to split. Now, although I have just shown two lines here to indicate the splitting that the splitting will involve, so as you bring say n atoms where n is a very, very large number to start creating a solid. This flitting will have a large number of finally, separated energy levels ok. So, the splitting will be very, very fine. So, you have you have the number of energy levels here being proportional to n. So, as we start bringing in more and more atoms you will have more, and more energy levels, and the splitting would be very, very fine.

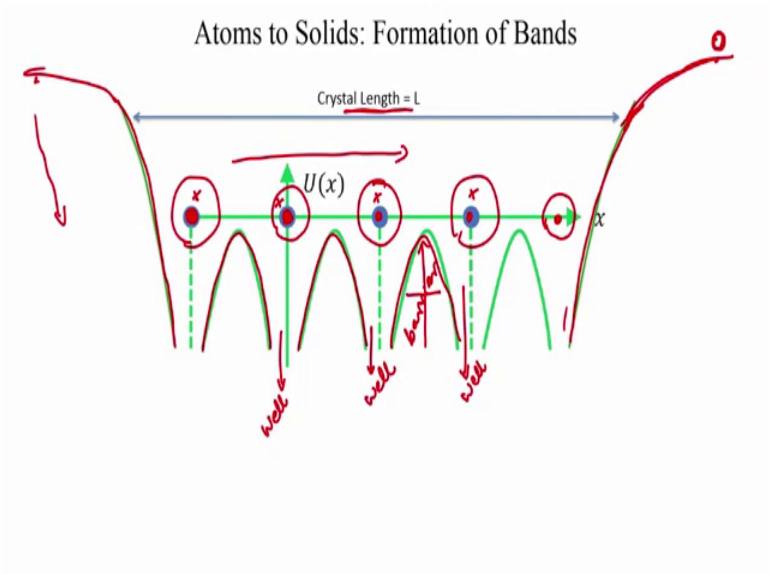
So, if we were to say, if you were to take this particular position, let us say the distance between the two atoms is this value here. And if we were to look at the energy profile, because of the system of two atoms, we would find that, this energy level would be quite discrete, I mean it would be almost single. There has not been much splitting in the innermost shell; whereas, the outermost shells have experienced significant splitting of energy levels.

And therefore, the outer shells would be would appear as bands of very finely spaced energies, very finely spaced energy levels and then we would have, and then we would have a very large gap, and these are the forbidden energies, because Schrodinger's equation does not prescribe solutions to the electrons. And then, we would have see another little band, another band which is again got very finely spaced energy levels.

So, this would be the energy profile that emerges from the experiment, where and we will start bringing atoms closer to each other. Now, what do we mean by energy levels, what are these dashes that, we are drawing here. Now, each of these levels ok, so the energy levels are nothing but solutions to Schrodinger's equation ok. And the electrons have to accept one of the solutions to Schrodinger's equations.

And therefore, these their energies are very specific and they are quantized ok and so each energy level basically provides it, it says that it is a spot that an electron could occupy, it is an energy state that an electron could occupy or in other words, it is a solution, it is a specific solution that they to Schrodinger's equation that an electron could take up. And these energy levels are also sometimes called as states or energy states ok. So, we imply the same thing.

(Refer Slide Time: 13:29)



Atoms to Solids: Formation of Bands

So, now let us look at a different picture ok. So, let us say we now, start we have brought in several atoms ok, and these are the nuclei the positively charged nuclei of all these different atoms. And we have arranged them, in a very periodic linear arrangement ok. So, you have these different atoms, and we have placed them in a nice periodic arrangement, which is just one-dimensional ok. So, we just have one dimension and along this dimension x, we have placed these atoms.

Now, the potential energy profile or the potential profile for each nucleus due to the positive charge of each nucleus would look like this. If I were to draw them all separately, these potentials would all appear like this and so on ok, so that that is probably another that is another nucleus here, that I have not shown. So, these it is only at the ends of the crystal so, let us say the crystal has got a length L. So, what do we mean by a crystal, we will define it more thoroughly later, but it is simply a periodic arrangement of atoms.

So, let us say this arrangement has got a total length L. So, we have now brought in 5 atoms, and there is a total length L and we find that these the potentials at these edges ok, as seen by the electron is would be 0, only at these edges. And the electron sitting here will be completely free from, completely free and would not know anything about this structure present here. But then as we get inside as we start entering this arrangement so, as we start looking at the potential profile along this a direction x. We will see that these potentials different potentials of these at different atoms. Now, interact and you will end up with a potential profile that looks like this, so you will see the potential starting to look like this.

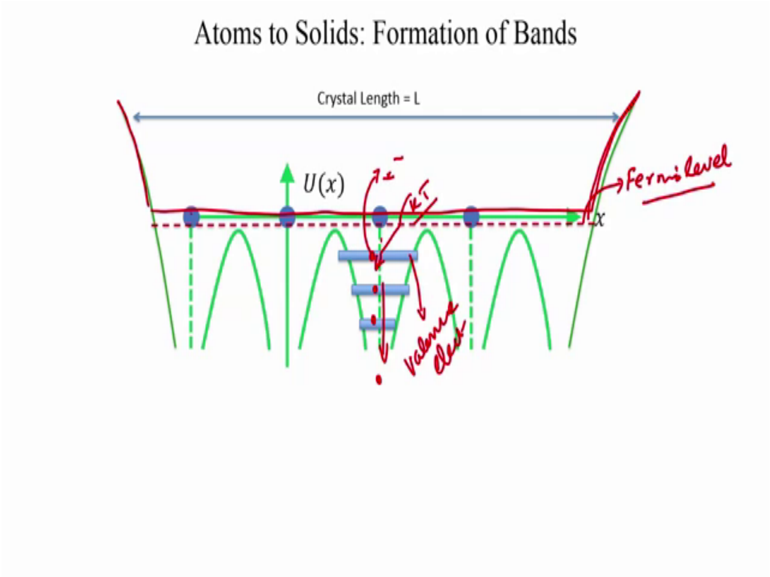
So, you have different potential wells, you have a periodic arrangement of potential wells, and you also have you also have some a kind of a barrier between these different wells, you also have a periodic barrier between these different wells. And, it is only at the edge, only at the edge of these crystals that the potential profile expands out in this particular manner.

So, this is the situation when you have a periodic arrangement of atoms in one dimension. And you could use, extrapolate this concept to any number of dimensions, you could say a three-dimensional atom, three-dimensional solid or a two-dimensional solid as well. And here we represent the potential term by U of x, so that is, that is going to be the potential that is going to take part into the potential energy term in any Schrodinger’s equation that we write.

So, now if you look at the energy levels the electrons occupy, so inside let us take this particular atom ok. So, inside this atom, the electrons are sitting in these discrete energy levels ok, which have now started experiencing some, some amount of splitting, because we have started bringing in many atoms closer to each other and the electrons that are least held by the nuclei ok. So, the so although the although, we have shown a blue circle there, it is only to indicate the presence of the nuclei it is not, saying that the nuclei is located there; in fact, the nuclei is located here. So, that is probably something I should have been careful about, so I do apologize, but I hope this is this is this is quite clear all right.

So, that is the blue circle they are just indicating the location of the nuclei ok, and this is the nuclei. So, all these energies, so as we head closer to the nuclei, all the electrons that are occupying energies closer to the nuclei are more tightly held by the nuclear. And it is only these electrons that are the most weakly held and they are something called as the valence electrons.

(Refer Slide Time: 18:03)



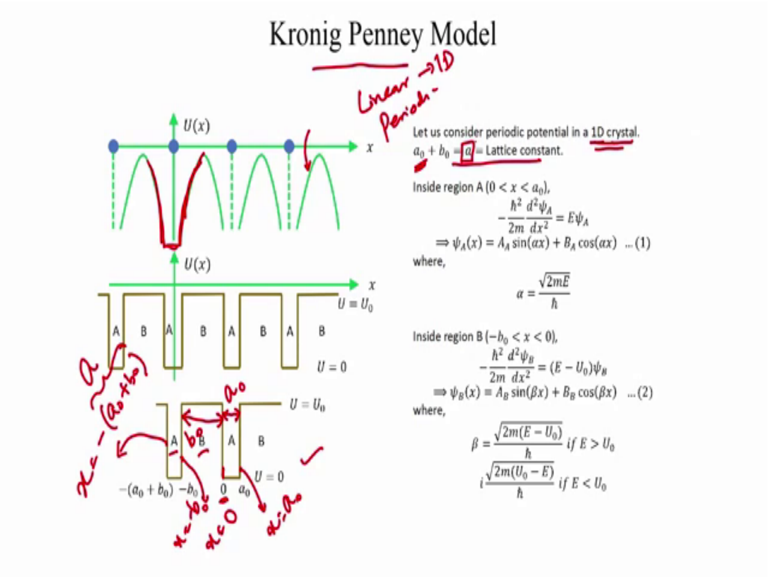
Atoms to Solids: Formation of Bands

And we have also indicated a red line here, a dashed red line. So, we will not worry about, the dashed red line for now, but this is something called as the Fermi level, and we will encounter the Fermi level later in this course. So, it is just something that is useful to know it is the Fermi level, and that is what this red line is. And we will encounter this term, and describe it more carefully later in the course.

Now, if an electron sitting in one of these atoms gets excited, let us say it receives a lot of energy either through either through an interaction of the photon or simply it just receives a lot of thermal energy, from the from a non-zero temperature in the ambience. This electron could get excited, and it could jump into energy levels that are higher up ok. And if these electrons could occupy energy levels that are above, above this Fermi level say for example, then one could say that the electron is now sitting in a different potential profile, the electron is now free to move out in the solid; and the electron now sits inside a potential profile that looks like this.

So, what this implies is that the electrons in this periodic arrangement see two kinds of boxes. So, we looked at particle in a box. So, the electrons here see two kinds of boxes, they see two kinds of potential wells. The first is the potential well prescribed by each atom, so this is one box and the second is if they were to escape the clutch of this atom, and enter into higher energy states; then the electrons would see a much wider box prescribed by the length of the entire periodic arrangement. So, now we are going to use all these ideas to develop a more mathematical and a quantitative estimate as with regards to the formation of energy bands, and energy gaps in a solid and all this is done via something called as the Kronig Penney Model.

(Refer Slide Time: 20:24)



Kronig Penney Model

Linear → 1D Periodic

Let us consider periodic potential in a 1D crystal.

$a_0 + b_0 = \boxed{a} =$ Lattice constant.

Inside region A ($0 < x < a_0$),

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_A}{dx^2} = E\psi_A$$

$$\Rightarrow \psi_A(x) = A_A \sin(\alpha x) + B_A \cos(\alpha x) \quad \ldots(1)$$

where,

$$\alpha = \frac{\sqrt{2mE}}{\hbar}$$

Inside region B ($-b_0 < x < 0$),

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_B}{dx^2} = (E - U_0)\psi_B$$

$$\Rightarrow \psi_B(x) = A_B \sin(\beta x) + B_B \cos(\beta x) \quad \ldots(2)$$

where,

$$\beta = \frac{\sqrt{2m(E-U_0)}}{\hbar} \; if\; E > U_0$$

$$i\frac{\sqrt{2m(U_0-E)}}{\hbar} \; if\; E < U_0$$

So, what is the Kronig Penney Model? To start off with our starting point is what we discussed, which is you have a linear ok. So, we say a one-dimensional periodic arrangement of atoms and these are the locations of all these atoms.

And therefore, you have a potential profile that looks like these green curves shown here, and as we mentioned the last atom that forms, that forms this linear arrangement would exhibit a potential profile that looks like this. And you could have electrons either being either sitting in these potential wells or they could be excited into higher energy states, and would basically experience a potential well that looks like this ok, which essentially means that the electron is free to move about in the entire potential well or the entire crystal in this case.

So, now to in order to start quantifying, quantifying this behaviour of electrons, we need to start solving Schrodinger's equation and since it is quite complicated to solve Schrodinger's equations for this energy, this potential profile, they are going to make a big assumption. And we are going to say that, we are going to they are going to say that yes, this is that this is indeed the true potential profile for seen by the electron in this linear arrangement of atoms.

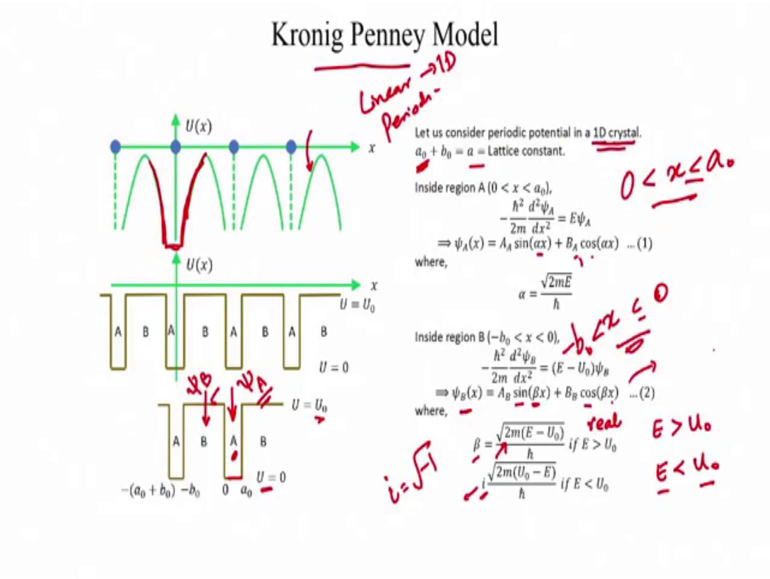
But we are going to make this assumption, and represent this potential profile by rectangular potential wells, because we know, we know the methods to solve Schrodinger's equation for rectangular potential wells. So, we say that, we say that, we got it, we are going to take we are going to take this true nature of the potential profile, and we are going to create a mimic or a model, which looks like this. So, it is a sequential arrangements of two regions A and B.

Now, A represents is indicative of this potential well here, so that is your A and B is indicative of this barrier. So, instead of having struck a geometry like this, we now have a very nice rectangular geometry and we also redefine our potentials. We say that this floor is now said to be the reference potential, and it is given by the symbol U which is equal to 0. And the barrier height is said to have another potential, which is given by this variable U naught ok, so we have redefined our potential energies so as to for it to be applied in Schrodinger's equation.

And further, we now consider two potential valleys, and we are just going to study these two valleys by looking at this picture here. So, we now redefine our x coordinates, and we say that this is the x axis, let us consider a sequential arrangement of A and B. And we will define the width of this potential well to have to be a naught; and the width of this barrier to be b naught. And we define the origin to be this location here the x is equal to 0 and we define, this point here as x is equal to a naught, and we define that point there as x is equal to minus b naught; and therefore, this point takes a natural value of x is equal to minus of a naught plus b naught. And this term represents, represents the periodicity of this potential map, and it is given a very special symbol a, which is called as the lattice constant. And this periodic arrangement is something called as a one-dimensional crystal ok, we will redefine the crystal much better in a few slides, but you can just note that, this periodic arrangement of atom in one-dimensional is, is also referred to as a one-dimensional crystal. It could have been wiser, if I had used a different symbol, since I have already used a naught here, but this symbol a is quite often used to define the lattice constant.

So, given this structure, we can now write Schrodinger's equation. So, we define the wave function in the different regions. So, we consider this region which is from x going from 0 to a naught.

(Refer Slide Time: 25:26)



Kronig Penney Model

Linear → 1D Periodic

Let us consider periodic potential in a 1D crystal.

$a_0 + b_0 = a =$ Lattice constant.

Inside region A $(0 < x < a_0)$,

$0 < x \leq a_0$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_A}{dx^2} = E\psi_A$$

$$\Rightarrow \psi_A(x) = A_A \sin(\alpha x) + B_A \cos(\alpha x) \quad \ldots(1)$$

where,

$$\alpha = \frac{\sqrt{2mE}}{\hbar}$$

Inside region B $(-b_0 < x < 0)$,

$-b_0 < x \leq 0$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_B}{dx^2} = (E - U_0)\psi_B$$

$$\Rightarrow \psi_B(x) = A_B \sin(\beta x) + B_B \cos(\beta x) \quad \ldots(2)$$

where,

real

$$\beta = \frac{\sqrt{2m(E - U_0)}}{\hbar} \text{ if } E > U_0$$

$$i\frac{\sqrt{2m(U_0 - E)}}{\hbar} \text{ if } E < U_0$$

$E > U_0$

$E < U_0$

$i = \sqrt{-1}$

So, this particular region when 0 is less than x, less than a naught ok. And we say that we could say 0 less than equal to. And we could say that the way the wave function in this region is psi of A. And we then consider this region B here, where x is less than less than equal to 0, less than minus b naught and say that the wave function there is psi of B. So, please note that we have not defined the wave function in this region to be psi of A, it is not psi of A. It the wave function takes the form psi of A only in this potential well. And although this potential well here, is very similar to this potential well to the other to it is twin. The wave function there is not psi of A, but it is related to psi of A and we will soon see, what that relation is.

So, here we have these two regions psi of A and psi of B. And we are going to write Schrodinger's equation for this region, and this region. So, since we have already gone through several such examples, it is quite easy to see that Schrodinger's equation for region A, this particular region A is given by minus h square by 2 m dou square psi A by dou x square is equal to E times psi. The potential term there is 0; the potential energy is 0. And therefore, psi of A has got a very general solution, which is of the form A A, that is A in region A sine alpha x plus B in region A cosine alpha x is equal to psi of A.

Now, once again I apologize for not taking choosing these variables more wisely. So, here A is a constant coefficient, A of A is a constant coefficient; and this represents A in region A. And B of A is again a constant coefficient that is basically talking about it is value in region A and the term alpha is nothing but your square root of 2 m E by h bar. So, this is the general solution of Schrodinger's equation describing psi of A.

Now, in region B, in this particular region, we now have a potential term, which is not 0. So, the potential energy is not 0 and therefore, we now have Schrodinger's equation, which looks like this, which is minus h power square by 2 m dou square psi B by dou x square is equal to E minus U naught into sine B. And the general solution to this Schrodinger's equation is also of this form ok, but with the, but with two different possible cases. So, here you have the coefficients A of B and B of B that form the pre-factors to the terms of sine beta times x and cosine beta times x therefore, the solution is A B sine beta x plus B B cosine beta x is equal to psi B of x.

Now, what is beta? If my energy the total energy is greater than the potential energy, beta is given by this particular expression, and it is a real value, it is got a, it is a real number. On the other hand, if E is less than U naught, which means the total energy is less than the potential energy, we see that the wave function can exists, exist even in that particular region, and that is, that is why the process of tunnelling, and that is something, which is very unique to quantum mechanics. So, therefore, the wave function can exist and beta takes the value of a it is a complex number, where i here is square root of minus 1. And, if beta is a complex number, and the sine and cosines of a complex number will result in exponentials of a real number.