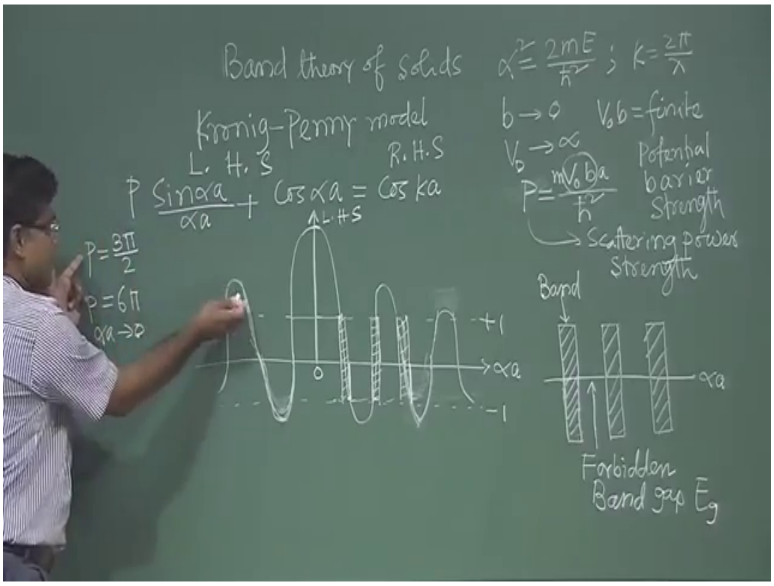
Solid State Physics
Prof. Amal Kumar Das
Department of Physics
Indian Institute of Technology, Kharagpur

Lecture - 43
Band Theory of Solids (Contd.)

So, we will continue our study on Band Theory of Solids.

(Refer Slide Time: 00:23)



So, from Kronig Penney model of periodic lattice periodic potential in crystal, assuming that the square potential with barrier which is b and potential is V 0; assuming b tends to 0 V tends to infinity, but V 0 b is finite. So, based on that we have got the condition for the valid solutions, this condition has to be satisfied. So, where alpha is I can write alpha is or alpha square is 2 m E by h cross square and k is wave factor k is wave factor basically it 2 pi by lambda and P, P is V m V 0 b a by h cross square hopefully its cross square yes.

So, that is the. So, we know what is b what is a, what is b 0. So, everything I have mentioned here. So, this P is you can see here it depends on V 0 b and V 0 b is called v is potential barrier and b is the width of this potential barrier. So, V 0 is called potential this it is called potential barrier strength. So, P basically depends on V 0 b. So, the P is called scattering power strength. So, basically electrons in lattice, there are barriers. So, what is the possibility of having getting scattered from this barrier, that is the P is the major of that scattering power of this barriers. So, here this P is very important parameter and I mentioned that from this condition we can get information about the energy momentum and many others things of an electron when it is in crystal.

So, I have drawn this one earlier in earlier class. So, here left hand side this is left hand side and this is right hand side. See if we plot here this left hand side this one as a function of alpha a. So, this restriction is that this left hand side has to be equal to the right hand side and right hand side value maximum value is plus minus 1. So, this value between plus 1 and minus 1, this left hand side whatever value will get. So, that has to be equal it cannot exceed plus minus 1 if exceeds.

So, that will not be allowed solution for this equation right. So, P you see here alpha a is a angle in radian. So, P has to be also in radian. So, if we take some value of P. So, in last class I took this equal to P equal to 3 pi by 2. So, you can take P equal to 6 pi; that means, when P value will increase for alpha a tends to 0. So, this term will be 1 and this term also is 1 so, but P is greater than one 3 pi by 2 or 6 pi by 2 ok.

So, 3 pi by 2 means it is 4.5 nearly 4.5; so 3.14. So, it is nearly 9. So, 4.5 P value is 4.5 this is one this is one; so 5.5. So, here alpha a this for 0 value close to tends to 0. So, its value it is around 4.5. So, this it will vary like this. So, this way it will vary because I think I should slightly smaller similar to this. So, this way this values. So, when this peak this peak value will reduce because alpha a are increasing alpha a are increasing; so P by alpha a. So, that is with this factor it will reduce so, but these value only those value are allowed which are within; so within plus 1 and minus 1 right.

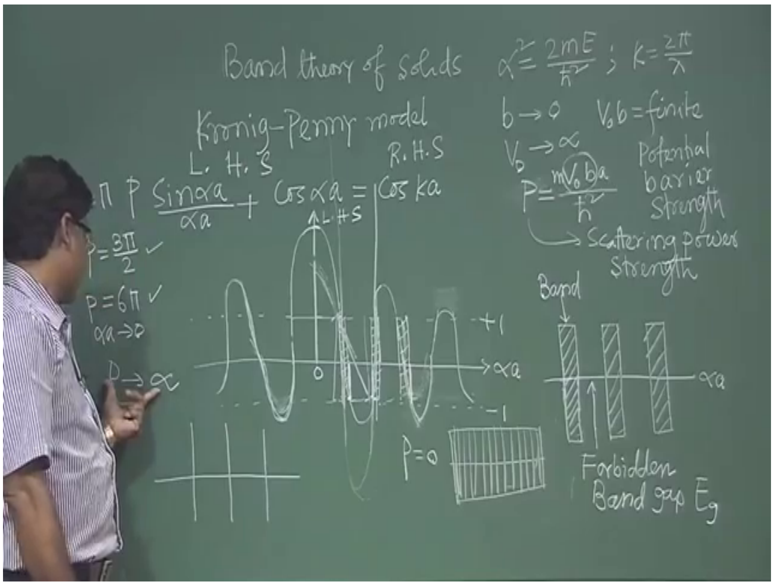
So, these are higher value then. So, these are not allowed these are not allowed for these satisfying this equation, only this part is within this range plus 1 minus 1. So, this value of alpha a, it is for this value of alpha a. So, this value only this value is allowed similarly here these value is allowed and this part (Refer Time: 12:02) like this. So, these value are allowed. So, as if. So, these are allowed value allowed region, these are allowed region, these are allowed region and other this part, this part is forbidden these are forbidden. So, this basically then we will get this type of alpha a, we will get basically this type of allowed region.

So, these allowed region we tell this energy, energy region because alpha, alpha a alpha is basically depends on a. So, it is you can tell that it is this axis is risky energy axis and.

So, this energy is allowed for electron in a crystal and this region are not allowed. So, these are called band, band energy where electron can and stay and these are called this region is called this forbidden region. So, it is called forbidden region between 2 band energy bands. So, it is called band gap it is called band gap. So, it will have some energy.

So, once can find out equating this with this relation in terms of energy one can tell this band gap energy value we express by Eg. So, here that is fine. So, here one can you can see if. So, I have taken P equal to 3 pi 2 if I take P equal to 6 pi by. So, what will happen? So, these will start this value will be I think this will be 16 approximately 16 earlier it was 4.5. So, it was 16. So, almost four times higher, these curve. So, basically these curves will fall sharply. So, this curve will fall sharply from here this way it will fall sharply, right.

(Refer Slide Time: 16:27)



So, high value then it is a. So, its variation will be its full very sharp when this value will be smaller say equal to pi. So, this now it is 3 point it is around 3.14. So, it will be it will start from here. So, it will be more broaden. So, it will be more broaden, it will be it will broaden these kind of variation you will see so; that means, this when P value is controlling basically this this slop of this of this curve, between these plus 1 and minus 1 so; that means, if it is the curve here. So, allowed value will be this right. So, it will be broader and when P value is very high. So, it will be sharp. So, allowed region will be just like a line right allowed region will be just like a line.

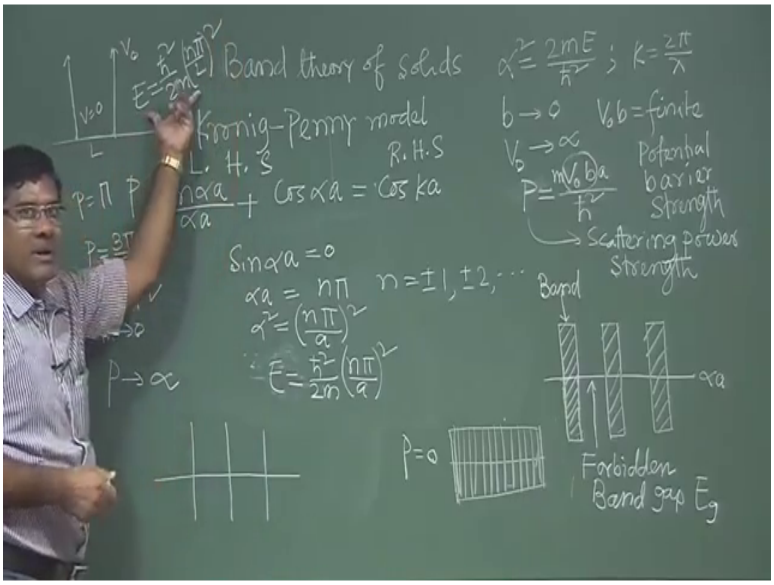
So, one can show that when P tends to infinity will be high value. So, you will get instead of this type of spectra you will get or P equal to infinity, you will get basically line spectra you will get basically line spectra and when P equal to 0 then what is happening. So, this P equal to 0. So, then cos alpha a equal to cos k a. So, this variation will be simply cos function. So, this function will be always between plus 1 and minus 1. So, all alpha a value are allowed all energy will be allowed right.

So, this variation will be within this variation will be within plus 1 and minus 1 plus 1 and minus 1 right. So, all value are allowed here it was not allowed because which part was not allowed which was going out from this value plus 1 and minus 1. So, that was the forbidden now no part is going out. So, all value are allowed. So, for this for P equal to 0 for P equal to 0 whatever you will get this energy that spectrum. So, I can draw it. So, it will be say here whether I can draw or let me draw here.

So, between plus 1 and minus 1 all value are allowed all value are allowed its continuous its continuous all value are allowed is if it is free electron is free to have any energy see its free electron completely free electron and in this case when P is infinity. So, this is strongly bound with the system. So, it is tight by link model also people call tight binding model and this P tends to infinity let us forget model. So, when P tends to infinity. So, it is just like discrete energy level as we have see for atom electron in atom, ok.

Electron in atom because this is the discrete because the electrons are strongly bound with the nucleus right. So, here these types of things are happening. So, its barrier is very strong mean means the electron is strongly attracted by the by the lattice ions. So, in that case we will the discrete energy. So, let us see this 2 extreme case when P tends to infinity and P tends to 0 when P tends to infinity you see this this term will be infinity, but it cannot be more than plus minus 1.

(Refer Slide Time: 22:07)

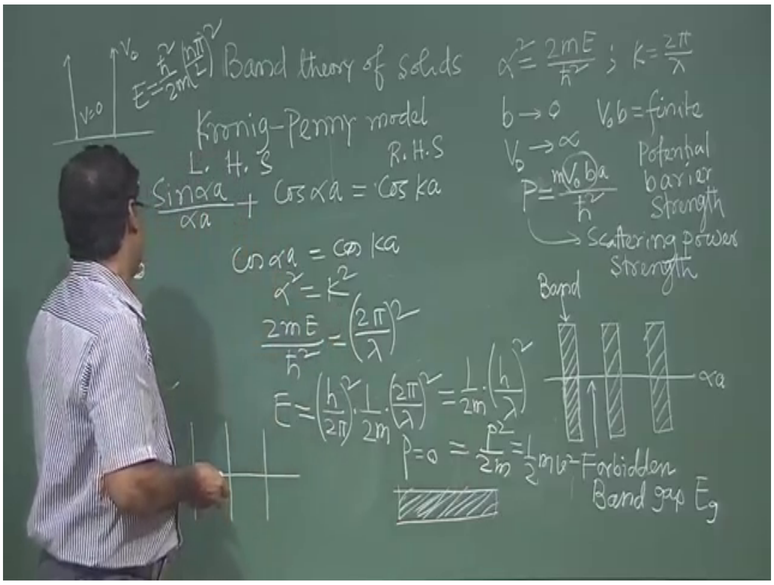


So, then this one can consider that sin alpha a has to be 0, sin alpha a has to be 0 right it has to be 0 so; that means, alpha a equal to n when it will be 0, when it is n pi right so; that means, alpha equal to n pi by a n pi by a; n equal to plus minus 1 plus minus 2 etcetera.

So, alpha is if square it alpha square equal to this square then alpha equal to any by plus square. So, equal to this. So, I can write E equal to I can write E equal to h cross square by 2 m n pi by a whole square right. So, so far, it is a things will get now we see that I think you will remember that in case of potential l right electron in a potential l here v equal to 0, but here v equal to say V 0, V 0 is very high see in that case. So, electron in a potential L in that case what was the solution? If it is this lane L right that solution was E equal to h plus square by 2 m n pi by L square.

So, if you remember this one that we have derived earlier, which at the beginning of free electron theory considering the electron in a potential L, only from the surface of the crystal this electrons are barrier, but inside potentially 0 or constant in that case which here type of (Refer Time: 25:02) . So, we got the same solution with the periodicity of a L lattice periodicity and here arbitrary L we can see that so, but the that was the length of this our potential L, periodic potential in lattice periodic potential in lattice. So, this potential are at periodicity is a and when this potential is very high, high I is infinity tends to infinity P tends to infinity. So, when potential is very high. So, we are getting this. So, as if these electrons are strongly bound in a system in the system. So, so that is why this we got this energy levels here also you got the energy levels right discrete levels. So, no concept of band electrons can stay in discrete energy level say here also similar this discrete energy level solutions are same, ok.

(Refer Slide Time: 26:43)



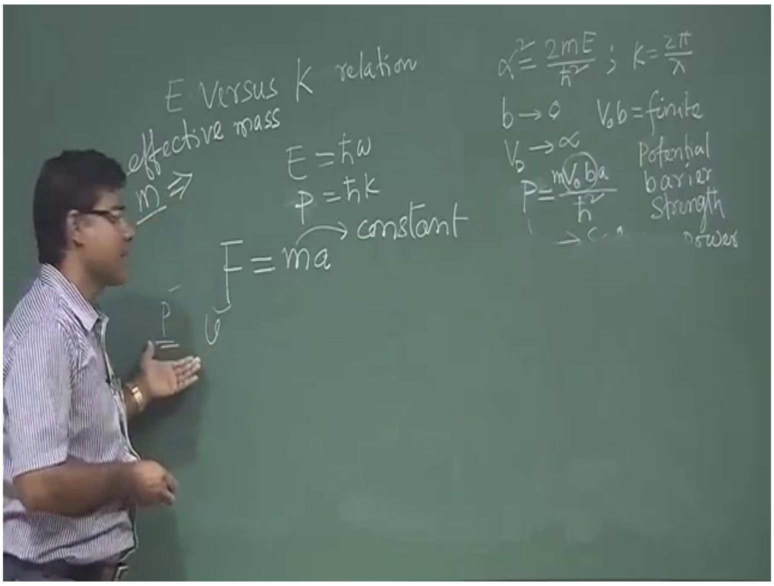
Now, when P equal to 0; so what we will see this I call it as P equal to infinity when P will be 0, P equal to 0 then this part 0. So, then we will get cos alpha a equal to cos ka right cos alpha equal to cos K a; so basically alpha equal to K alpha equal to K, right. So, alpha is; alpha square k square alpha a square is 2 m E by h cross square equal to K square is 2 pi by lambda whole square right. So, I will get E equal to. So, h plus square means h by 2 pi whole square h cross square left side then I will get this 1 by 2 m and then I have 2 pi by lambda whole square right. So, 2 pi square it will go. So, what I will get?

So, h; so I can write. So, this 2 pi, 2 pi square 2 pi square it will go and then here h square and this one by lambda square. So, I can write h by. So, 1 by 2 m, 1 by 2 m h by lambda whole square right, but I yes. So, h by lambda is electron. So, one can treat as a wave de Broglie wave right. So, this is h by lambda is p. So, this is basically h square by 2 m. So, P square by 2 m energy is P square by 2 m this is our free particle its half m v square we can write half m v square. So, this energy expression is telling as that its electron free. So, when P equal to 0 its telling that electron is completely free when P equal to infinity electrons are strongly bounded in the system.

So, that is how this when I draw the for this case P equal to 0 as I draw there, that is allowed energy level of continuous all energy. So, electrons are free in the lattice. So, that is the free electron. So, this P is the basically very important parameter which can give or whether tell whether electron is free or whether electron is loosely bound or electron is tightly bound.

So, now question is that this depending on free value whether electron is free whether electron is tightly bound.

(Refer Slide Time: 30:47)



And its energy relation are different energy relation energy of the electron will be different depending on the situation of the crystal of the situation of the potential of the of the crystal, right.

So, for free electron what is the energy? So, basically in energy versus K that is important relation energy versus K important relation for free electron energy you have seen that I think one can write energy equal to h cross omega and K one can write no P momentum P one can write h cross k. So, for free electron that for energy and momentum relation is there now in case of crystal when the electron is in crystal and it is not free. So, what will be the relation of P and K. So, that we want to find out second thing is that what about the mass and momentum and velocity of a electron in crystal.

So, for free electron its (Refer Time: 32:36) to the notion. So, acting force on that from the system from the electrons. So, we can write m a and m is constant of the electron or of the particle right whenever we have applied force. So, if the acceleration will change velocity will change, but it is the mass constant.

So, in these case when that electron is in is in crystal with our it is mass is constant or mass varies that is one important fact we have to we have to see. So, we will see that n is not constant n is varies even m become negative. So, that is why we tell this that mass of a electron in crystal, that is effective mass and will see that m even become negative and velocity whatever the velocity in the crystal or momentum in the crystal momentum in the crystal, ok.

So, that is also different whatever the free electron whatever this momentum and velocity it is in when that electron is in crystal its momentum and velocity also is different, its behaviour is different it completely depend on this e versus k curve or relation. So, that is a e versus k relation is very important first we have to find this relation. And then we can answer of this question what about the mass what about the momentum and velocity in crystal.

So, I will discuss those things in next class.

Thank you for your attention.