Solid State Physics
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Lecture - 42
Band Theory of Solids (Contd.)

We will continue our calculation.

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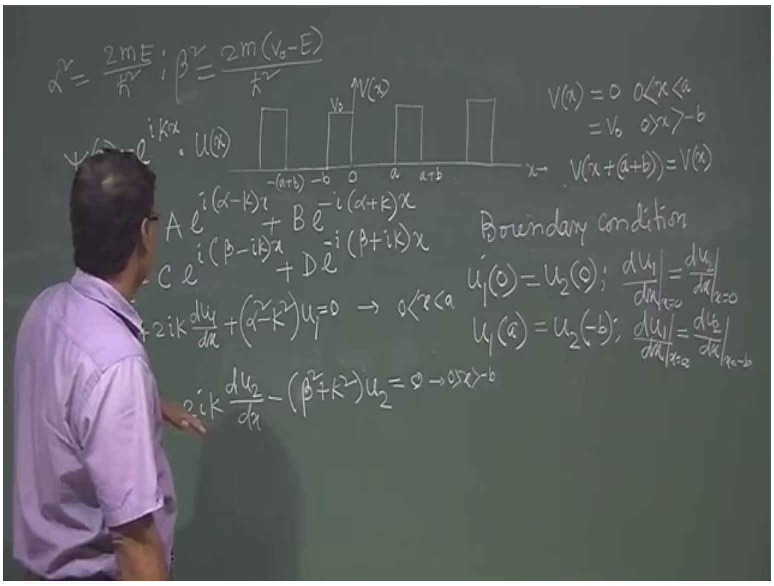

These are the boundary condition. So, whatever I am doing, the just method, you will do this type of calculations many times in quantum mechanics. This is the method this way one has to proceed, now you see at use boundary condition, I think I do not need this one now from there I can yes, I have this, these are the trial, these whether I will need later on.

These are the 2 solutions we have written for these 2 equations is the general solution now you have to add up with our system, that is why we have to apply boundary condition. So, if I apply boundary condition what you will get, u1 0 equal to u2 0, u1 0 means x equal to 0.

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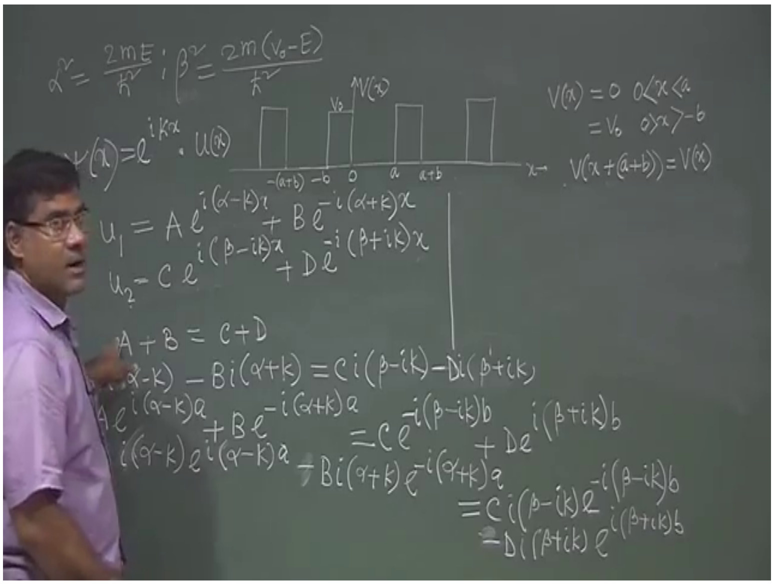

If I put x equal to0, these will give A plus B equal to C plus D, for this I can write and then this one we have to differentiate and then we have to put x equal to 0. If I differentiate, this i alpha minus K that term will come out, what I will get A i alpha minus K right e to the power this, x is equal to0, it is one I will get this.

And this one if I differentiate minus i alpha plus k, this plus is there, it will be here minus and will get Bi alpha plus K, x equal to 0. I will get this equal to same way I will get Ci beta minus i K, here this plus, it is minus, I will get minus i beta plus i k. Then D of course, D has to be there, D and then this is minus sign, so that differentiation after doing differentiation putting x equal to0, then this from this condition what I will get. So, x equal to Ai have to put an x equal to minus Bi have to put here.

What I will get A e to the power i alpha minus K and then x equal to a then I will get this one plus B e to the power minus i alpha plus k a equal to I will get equal to I will get or minus b, x equal to minus b u 2. I will get C e to the power I beta minus i k right, x equal to minus b, minus here I can write b here right plus D e to the power minus, this is minus b so, minus plus, I will get i beta plus i K b.

And then we have to differentiate and then x equal to a, for this and for other one x equal to minus we have to put. So, basically whatever I got this condition, only when you will differentiate these parts will come out this part additionally we have to put, this part is nothing, but you can see this part for this part it is this or this part it is this anyway. So, what we will do just here A e to the power i, if differentiate A then I will get i alpha minus k right now this will be there. So, I have to write e to the power i alpha minus k and this is a right. This is one term plus B, when you will differentiate, this part will come, it will be minus B i alpha plus k then this term will be there. I have to put A, e to the power minus i alpha plus k a, equal to for C same thing I have to do for this side, differentiate it. It will be C i beta minus i k now x equal to minus b, I have to put e to the power minus i beta minus i k b, minus b, minus I have taken here.

Similarly I have to write for d part, but I need space, plus here probably I can write yes plus D, differentiation these part will come out, it will be minus D i beta plus i K, then this term I have to put minus b, it will plus, e to the power i beta plus i k b. Here you see this 4 equation I got I have 4 unknown if you solve them, basically you will get the value of A B C D, but it is, generally what people do, take the determinant you see A is coefficient of A B C D, I can form a determinant. So, think I can from here, but it will be right, I can form determinant how just coefficient of, the coefficient is one here, one here, one, one right.

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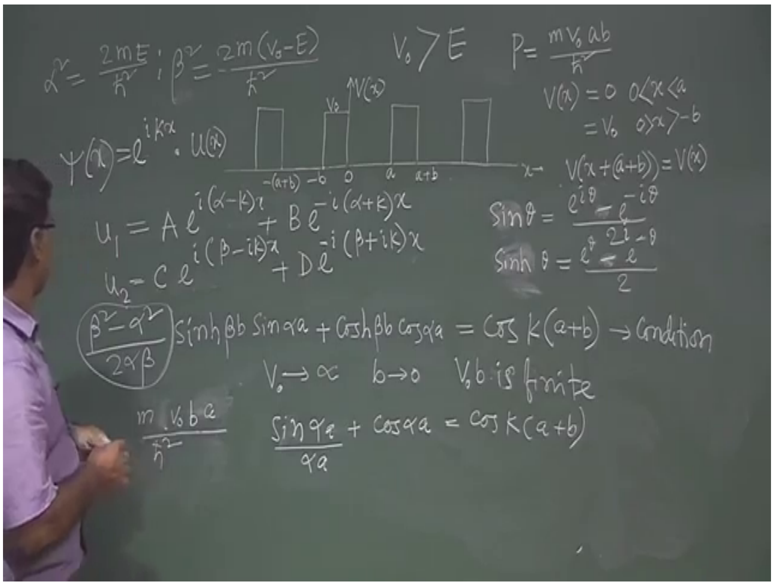

So, for from these coefficient is this from here this coefficient i for this i alpha minus k alpha minus k here coefficient of B is minus i alpha plus k right, coefficient of C I can write i beta minus i k, coefficient of D I can write minus i beta plus i k. Similarly, here coefficient of A, this e to the power i alpha minus k into a, coefficient of B this coefficient also I can write, I can write, I will not write. So, just one has to from here one has to write similarly from here coefficient of, 4 column 4 row determinant 4 by 4 determinant. Now, condition is when you use determinant condition is if this equal to 0, then if this determinant vanish means this determinant is equal to 0 then it will give non vanishing coefficient and corresponding wave function will get.

The condition is to serve this equation and getting the meaningful non vanishing solution, this determinant has to be 0. So, now, one has to calculate it is it is time taking, but you should once you should calculate one has to see to this lengthy calculation that is I think I do not need to do here it is you can do yourself it is quite lengthy and one has to see to it and do this calculation. I will just write the result if this determinant is equal to 0, what you will get, you will get basically just solving this I will get beta square minus alpha square by 2 alpha beta sin hyperbolic beta b sin alpha a plus Cos hyperbolic beta b Cos alpha a, from this determinant you solve then finally, you will get this type of condition that will be equal to Cos K a plus b.

Let me check whether I have written correctly alpha beta, these will be the solution of this determinant now here I think you are familiar with these sin hyperbolic Cos hyperbolic hopefully you are familiar. So, these let me tell you Cos theta equal to e to the power i theta plus e to the power minus i theta divided by 2. So, Cos theta, Cos hyperbolic is theta is basically here itself I can e to the power theta plus e to the power minus theta divided by, this when this complex this i is not there just one has to remove this complex side. So, that function is called hyperbolic function, similarly for sin theta you know this if I write this sin theta, this become this is minus and this 2 i because e to the power i theta equal to Cos theta plus i sin theta, from there one can get it, similarly this one for sin hyperbolic, this will be just minus.

This is the definition of this hyperbolic function, that is, this type of things was in our equation e to the power the term was there with i without i so, that is why this term has come. Here, this is the solution we got, this basically the condition and this condition has to satisfy by this system, what is beta square minus alpha square beta square, what will do now, this is also looks complicated right. Now, we got the equation expression mathematical expression, but our aim is to use this expression to explain physics. We have to try to make it simpler, Kronig Penney consider that if V 0 tends to infinity and b tends to0, but V 0 into b or is finite.

So, b tends to 0 means this is the right, b tends to 0 means this width of this barrier is small and b tends to infinity means this small and this potential is this very high, under this condition then we can simplify, beta square minus alpha square, minus of this one right. It will be 2 e what we will get this term from, this term we will get beta square minus, 2 m b 0 minus 2 e divided by h cross square and then we have 2 alpha and beta.

Basically, this 2 we can remove and if we consider this condition V tends to infinity means V is very high compared to e and one thing I did not mention in earlier class probably I mention that here I wrote V 0 minus e because we consider that v 0 is greater than E, we are solving this problem considering V 0 is greater than E, because these electrons are confined in this potential if V 0 is less than E, electron this barrier can easily can overcome, it will be equivalent to free electron.

This is the condition, if V is very high compared to e, I can remove this, m V 0 I will get m V 0 by h cross square alpha beta from here now here what I want to do and this term theta b, beta b tends to 0 right, this term beta b, beta b will be tends to 0 then what we will get, we will get this small value. So, sin theta if small value, that equal to we can write theta sin x equal to expand it or small value.

It will be approximately theta right, this term I can write, sin hyperbolic beta b, sin hyperbolic theta equal to theta. This one can write beta b, since these are small value because as per this condition, so then I will get here this and then sin alpha a alpha a plus this will be beta b tends to 0, Cos 0 it will be for small value, it can be written one. I will get basically this is one under this condition beta b tends to0, I will get Cos alpha a equal to Cos k a plus b.

This is the things I got now what I will do, this is beta will go, b part will be here right, I have written right now what I will do I will just multiply with a in denominator and numerator, so my m is to make it like this, this alpha a here I want to put alpha a right, in this form alpha a I have taken this now this m v 0 a b by h cross square. So, this I am writing just one parameter say P, P equal to m v 0 a b by h cross square, this parameter is very important because here v 0 b is there and this assumption we have made here v tends to infinity b tends to 0, but b 0 b is finite.

We will see the effect of this parameter P, P is this, I can write, I think I do not need them now, so we have simplified this one under this condition. And finally, what we got, we got P sin alpha a by alpha a.

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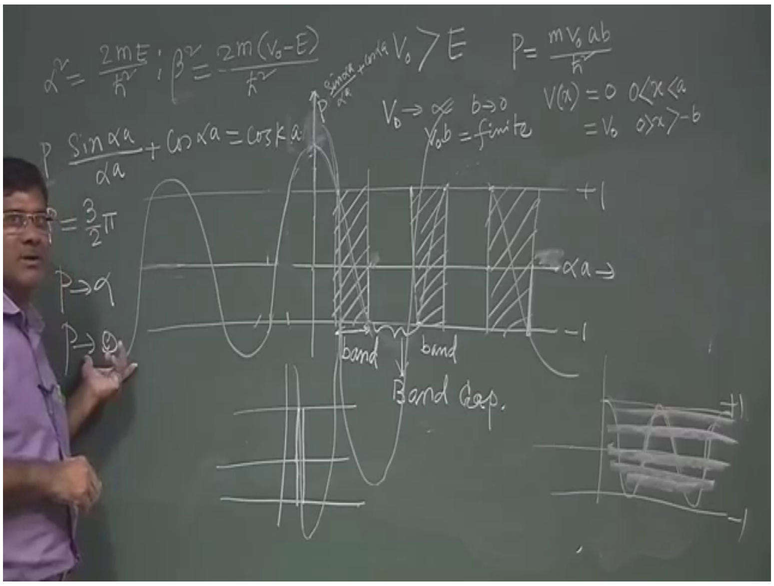

Plus Cos alpha a equal to Cos k a plus b and for this condition we have taken a condition we have taken I do not need this also condition I have taken V 0 tends to infinity and b tends to 0, but V 0 b is finite, under this condition we got it, this simplification is made by Kronig Penney.

Now, you see, what will be the P value it is you see this is a angle right Cos something this Cos these and this sin this, so this alpha a or whatever these are basically in radian, alpha a also it will be radian right. Here or if you see the dimension, sin and Cos terms p by alpha a, whatever the dimension this one, this p will be have the same dimension right. P also basically one can write in terms of some angle in radian, if I take P equal to some value say 3 by 2 pi and then for this value if I plot this equation if I plot these.

So, what it is telling, I will plot alpha a and also I need some more I have to make it more simplify I have to simplify more here also b tends to 0, then I can remove this b, this is basically Cos k a. Now, if I plot say left hand side if I plot, here in terms of alpha a if I plot and that is that this part will be equal to that other part and Cos value it can have maximum it can have value between plus 1 and minus 1 right. So, these value cannot these value has to be also within the range plus 1 and minus 1.

Let me draw those 2 line one is plus 1, 2 boundary and another is minus 1. If I plot this one, this has to be within this range right, but if I plot here you see, at this is 0 axis I have taken now if alpha a tends to 0, sin alpha a by alpha a. So, this is one limit alpha a tends to0, that is why I have write in this form, at 0 it is one, what about the P value 3 by 2 it is just we have taken you can take in the other value also.

It will have value, these values definitely it is higher than the one right see it is almost 4 to 5 times of one, it is value is here, I think I will, it is value is here. So, this one is this function this along this axis basically P sin alpha a by alpha a plus Cos alpha a right along this we are plotting. If you plot, you will get basically here this type of things you know, at alpha equal to 0 it will have maximum value, these part will be one this is one and this part will be plus this basically. So, equal to this side forget, now, if alpha a is increasing, this value cannot be higher than one right, but this value is increasing and then this term will decrease this term will because P is constant here, this term will decrease, mainly it will follow this term, I can, what I can do, I will get this type of variation, for higher value of alpha a, this will decrease.

Now, what will be solution, this side, basically this, whatever value it will be between these two and for this function it is varying like this, solution has to be within this right. This outside of this cannot be solution cannot be point accepted which forbidden right, what will happen, from here to here, this is our, this function and it is guiding us that it has to be within this plus 1 and minus 1. This part will be the solution if it will satisfy this equation similarly this part is not cannot consider it will not satisfy this condition, this part again. These are the solution other part will not be the solution. So, here I can, basically this region this region is allowed this part is allowed right, this can be the only solution.

Similarly, these parts will only the solution because this part only within this plus and minus, other part this part is see more than plus 1 this part is more than minus 1, these are not allowed. This part only the allowed part similarly here also one can show, the one can draw, but anyway it has to be it will (Refer Time: 36:01) symmetric. One has to draw properly; I think this I have not drawn properly. Anyway I think I should, but forget it. So, other side also one can get this type of allowed region, this part is allowed and this value you can see this value, when wave function was going this Cos function, this is minus, Cos when it will be minus.

So, for pi value it will be minus, that is why this point I can write pi alpha a is pi and then, this is the wave and from there you will get, this will be 2 pi sin alpha a it is or Cos 2 pi is one sin alpha a 2 pi it will be0. This way one can I think I have drawn this that is why I am facing problem, pi 2 pi where is pi this is pi where it is going it is going this is coming it will be plus 1 for 2 pi it will be plus 1.

This say one has to, this will be I think I do not know, anyway, pi 2 pi etcetera one can, better I will not put something confusing to me any way, what we have seen here, this is the allowed region and this is the forbidden region, within this, whatever the this you see this what is this, alpha a whatever is alpha is basically here is E. So, this is basically energy scale right, these energy are allowed, these energy are not allowed these energy allowed.

This basically is called band it is called bank, here only this energy this is the energy are allowed electron can stay here in this region, in this region electron are not allowed, it is called band it is called forbidden region. So, it is called, this another band another band, between 2 band, this is the forbidden region, this is called gap band gap. So, I think I have to stop so, but it is very interesting, in next class I think I will take this equation and I will tell about more. So, just I can tell also now if I take this higher value of p, p tends to infinity, what will happen, this terms is infinity right this term looks infinity or p is higher and higher, this edge will be sharp this edge is falling here, it will fall sharply, it will fall sharply.

That means when it falls sharply, between one and minus 1, you see this is the allowed region, you know this is the allowed region, this band width will be very small it is very very small. In fact, when it is tends to infinity, it will be just one line, it is tends infinity means tends to infinity means this is V 0 a V 0 b is this tends, b tends to infinity means this width will be tends to 0 and v 0 tends to infinity see it has finite value, but what is happening, I will get just like a one line right.

So, that is the energy if level as we are seen for atomic case because it is this potentially so high; that means, the electrons are confined in there it cannot move see it is just like energy level will get, band will converge to the energy level just one line. Now other way if P tends to 0 then this part is not there, it is just Cos function, it will vary like this 0 Cos alpha 0 Cos alpha is 0 means this is one, it will vary like this. So, all the time this value will be within plus 1 and minus 1.

So that means, all value are allowed all value are, this continuous, all energy all energy are allowed it is just like free particles there is no energy level it is continuous, it is just free particle. When P value is small tends to 0 it is just behave like a free particle there is no potential and when it is tends to infinity it is very hard barrier and for very hard barrier, electron is confined like the atom, you will get just sharp energy levels, then will not be there now in between 0 and infinity whatever is value will take, there you will get band and gap between these 2. This complicated mathematics not complicated lengthy etcetera one has to simplify.

And finally, we are getting very interesting physics, one has to really understand, and hopefully I tried to tell you this physics out of this, this is the very interesting after long calculation. I will stop here.

Thank you for your kind attention.