Solid State Physics
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Lecture - 41
Band Theory of Solids (Contd.)

So, we continue our Band Theory of Solids.

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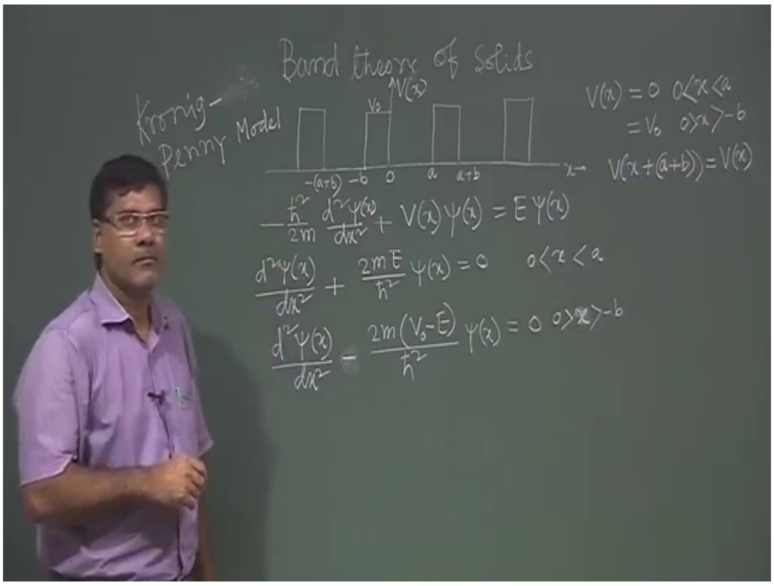

So, we have seen that in crystal lattice points are there atoms are there. So, if we consider one dimensional lattice. So, they are periodic potential one can consider, so these periodic potential right. So, this potential, it is basically as per Kronig and Penney as just I have discussed so that was the potential periodic potential one can consider for a for a crystal. And this height is V 0, and say if I take this axis V x and this is the x. So, this is 0, this is a, this is minus b, this minus a plus b, this point, and this point a plus b. So, there is a periodicity is a plus b, and that V x potential for this is 0 this is 0 for x is x is greater than 0 and less than a right.

And this V x is V 0 for the range x is less than x is less than 0, and greater than minus b. So, this is the periodic potential is considered for a crystal one-dimensional lattice, and this periodicity is a plus b. It should be b x. So, whatever potential say the x is equal to 0, so here whatever potential here. So, it will be at a plus b at a plus b, here it will be same potential or minus a plus b, it will have the same potential. So, that is the periodicity.

Now, one can just consider this middle of this, and middle of this. So, that can be the halves so that also a plus b. So, these are the potential that was considered by Kronig and Penney. So, that is why it is called Kronig Penney model. So, whatever now we are doing that is basically Kronig Penney model. So, for these Schrödinger equation we have to write Schrödinger equation h square h square by 2 m d 2 psi by d x square plus V x psi. Of course, function of x equal to e psi x right. So, this is the general time independent Schrödinger equation. And this is non-relativistic earlier I am not mentioned Schrödinger equation is basically non-relativistic equation. And relativistic equation that is in quantum mechanics that Dirac equation.

So, we have 2 region in one region this potential is constant V 0, and another region this potential is 0. So, you can we can have this d 2 psi x by d x square, then plus if it is d x if it is 0, then 2 m E by h cross square psi x equal to 0. So, that will be the one Schrödinger equation for the region x is greater than 0, and less than a for that region. Similarly, for other region d 2 psi x by d x square plus. So, this if you take this one this at could be 0. So, if take this other side. So, e minus V 0 so, but I want to write V 0 minus v. So, here minus sign 2 m V 0 minus e, divided by h cross square right psi x equal to 0 ok.

So, this is or this region x is less than, x is less than 0 or greater than minus V for this region. Now let us there is a constant let me write somewhere.

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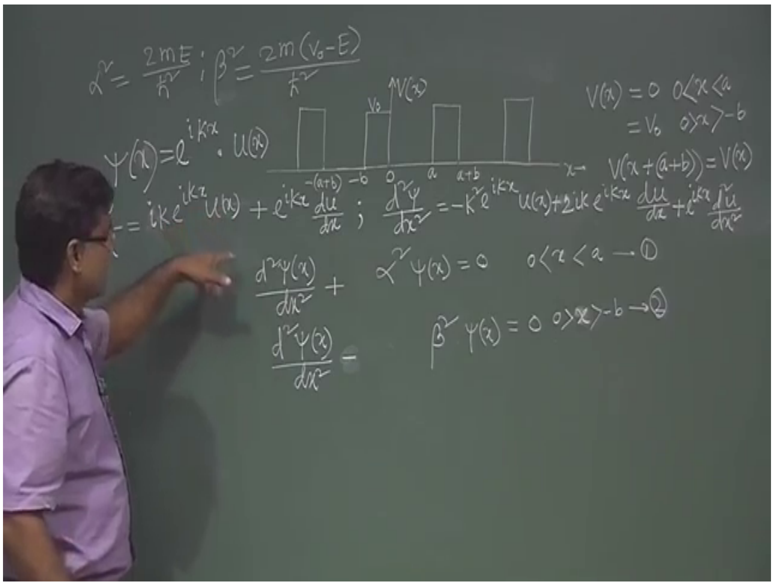

So, let us consider this alpha square equal to 2 m E h plus square. So, this is just like defining this one. So, this I can write alpha square then I will define beta square. So, let me beta square equal to 2 m V 0 minus e divided by h cross square. So, then I can write here beta square right.

So now here I have for these two region this 2 Schrödinger equation. So, say 1 and this 2. Now we have to we have to sub these 2 equations. So, for that what we do we consider the wave function? We consider the wave function, proper wave function we choose proper wave function so that so for free electron theory there e to power minus k dot r. So, in our case for one-dimension e to the power i case this planar if travelling wave. So, this so here it is basically free electron, but now we have introduced periodic potential right.

So, we can assume that so for free electron what are the wave function that is there as well as another wave function say u x. So, that u x one can introduce. So, this u x the potential that these type of arbitrary function looking at the our problem. So, this I am writing just it is guided by Bloch, it is guided by Bloch. So, Bloch he found that this for any periodic potential the wave function will have 2 parts one is this and this one is served at one part is travelling wave or plane wave, and that will be modulated with another function which follow the periodicity of the potential periodic potential. So, what does it mean? So, u x that will be such that u x it will be such that which u x pass this periodicity of this potential is here a plus b that will be equal to u x.

So, that is the property of this of this function. So, it also this function is periodic and it will have the same periodicity of these potential. So, this u x it is called Bloch function. And one can prove one can prove it that this type of wave function satisfy any periodic potential; so this so in our case of according to Bloch. So, we have to take this wave function. Now we have to add up this wave function without system applying boundary condition, and applying our this periodic potential condition so that we can do starting from this wave function. So, this now this is the say psi x our trial function some, it is called trial wave function.

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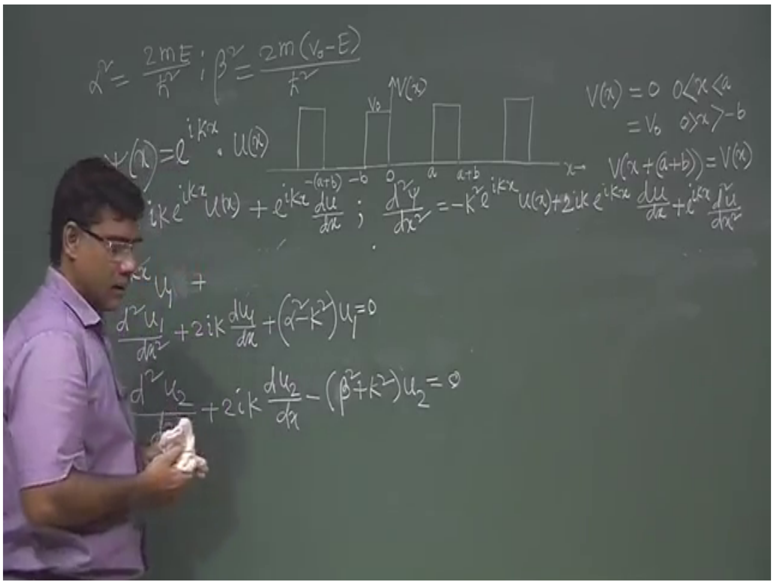

So, from these function I can write that, I can find out d psi by d x d psi by d x will be equal to e; so if I so i k e to power i k x u x plus e to the power i k x d u by d x; so then again differentiation d 2 psi by d x square.

So, this again you can proceed. So, this will give I think I will write here. So, I need space now if I write d 2 psi by d x square equal to this one. So, again i k I square minus 1. So, minus k square minus k square e to the power i k x then u x right. And then keeping i k e to the power i k x e. So, d u by d x; so now next part we will have here i k e to the power i k x d u d x. So, basically these term i k if this. So, I can put here 2 plus, e to the power i k x d 2 u by d x square, e to the power i k x d 2 u d 2 u by d x square right, d t u by d x square. See it is not visible I think I can it is going out; so plus e to the power i k x d 2 u by d x square right d u by d x square.

So now, I can replace here what I can get from these? Here So, just for these 2 equations. So, this periodicity here this we can let u we can take this travelling wave now this modulated with this u. So, I can consider for these and equations for this one. So, here I can (Refer Time: 19:08) e 1 and this other one is u 2. So, I can write. So, I can replace this 1 by this and is. So, what I will get? I will get minus k square e to the power i k x plus 2 i k sorry. So, here I will write e 1, it is a function of x of course, and then plus 2 i k 2 I k. So, I am replacing this part 2 i k e to the power i k x d u 1 by d x and then plus part plus e to the power.

So, this will be there alpha square i x. So, I will write later on. So, this e to the power i k x d 2 u 1 by d x square right, plus alpha square psi x means this one e to the power. So, this also I have to shift, this 1 plus e to the power i k x e 1 e 1.

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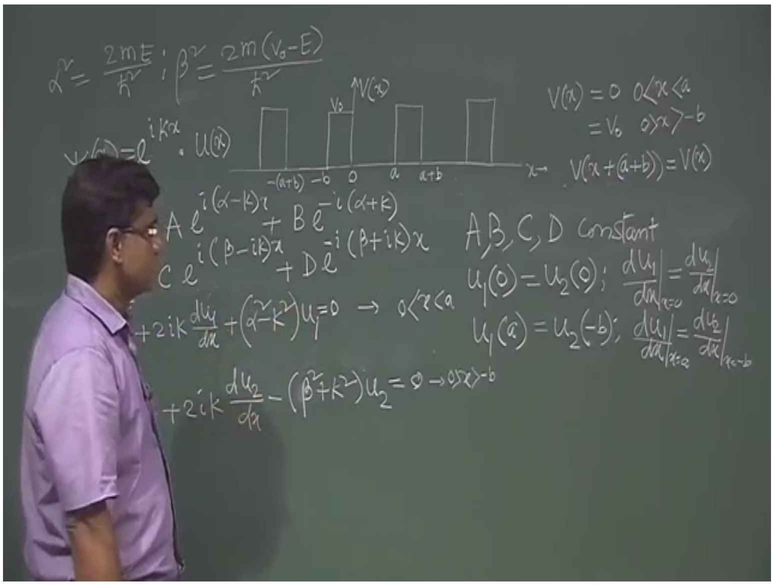

So, e 1 it is function of x I am not writing this one just e 1 I am writing, this equal to 0. So, this is for that region x is greater than 0 and less than a. Now for this part; so here you can see I can write. So, a b term contains it is not plus alpha square psi x y. So, it is alpha square I think it is just alpha square. So, basically you can remove this from which term, and then what else are common? I think then you can we can write this d 2 u 1 x square d 2 d 1 by d x square, this term I have written this term I have written. And then this term d u 1. So, plus 2 i k d u 1 by d x d u 1 by d x, and then I will have I will have this term so here.

So, this I have to d 2 psi by d x square minus this. So, then I will have alpha square minus k square right, e 1 equal to 0. So, for another part, for another part I will get similar one only difference is earlier it was plus alpha square psi x, now here minus beta square. So, minus sign is there. So, I will get same way d 2. So, in this case u 2, but this d x square plus 2 i k d u 2 by d x square d x plus. So now, it is beta square right. So, minus k square it is there now minus beta square basically minus alpha square minus beta square plus k square. So, I have taken this minus sign u 2. So, that is equal to u 2.

So, that is for 2 region, these 2 are for 2 region. So, so I think I got the right one yes. So now, now here what we have to do I think this also I do not need yes. So now, we have to put boundary condition. You have to put boundary condition that here you can see this part is basically is equivalent to alpha minus k into alpha plus k. Here this term is equivalent to beta plus i k beta minus i k right. So, beta square minus i k square. So, I square will be minus 1 so that way plus k square.

So, here this is second order differential equation. So, from here you will get basically 2 root, see if you have 2 root, so then your general solution. So, 2 root means for u 1 you will get 2. So, what about this nearly what I want to mean that e to the power say m x or I m x whatever if I consider on a one solution for u; iIf I put here if I put here. So, this second this is the second order differential equation. So, I will get basically here you can see m square etcetera

So, m I have to find out m square this will be then this will if one. So, this so from here you will get value any value is something plus minus something. So, you will get basically 2 value. So, this true value basically from here one can one can guess. And general solution will be that the sum of this 2 or 2 wave function. So, if is has 2. So, say m one another you will get I n 2. So, general is written a if this equal to a this plus b.

So, that is the principle of second order differential equation. So, following that one we can we can take we can take this general solution for u. So, this for u 1 if I take general solution for u 1, u 1 equal to a e to the power i alpha minus k x plus b e to the power minus i alpha plus k. So, so these 2 terms as I mentioned I have taken from here and for these u 2. So, I can write c e to the power i beta i k or k i beta so whatever. So, I will write in my case; so this one i here so beta minus i k. So, I think I should write below slightly below I should write. U 2 equal to c e to the power i beta minus i k x of course, will be there plus d e to the power i minus i beta minus plus i k, ok.

So, this I can consider this is a general solution, but it just does not matter because this I have to put here. And this should satisfy these and then proper form you will get. So, this is just general form, but as I mentioned this one should look at your problem and try to construct guess say better function. So, there will not be much complication to reach to your particular solution.

So now this a b c d are basically the constant. A b c d are basically the constant, these are constants. Now this value of this constant one can find from the boundary condition right. So, what are the boundary condition? I can say that boundary condition u 1 at 0 because function has to be continuous. So, u 1 at 0 equal to u 2 at 0, so both value should be same for at x equal to 0. And their differentiation also has to be the differentiation also has to be d u 1 by d x at x equal to at x equal to 0. It should be equal to d u 2 by d x at x equal to 0.

So, this is the continuity, this is the continuity of wave function at the at this point. And this it has it has to also satisfy this periodicity, this periodicity. So, so this u 1 at a u 1 at a has to be equal to u 2 at minus b, whatever here. So, it has to be same as minus b. So, why I am writing minus b or why this one because this because that this equation. This is for x is greater than 0 less than a and this for x equal to less than 0 and greater than minus b right. So, when u 1; so I have to take within this rage. So, u 1 a at this point. So, that has to be same as that u 2 at minus b ok.

Similarly, is their differentiation d u 1 by d x at x equal to a has to be equal to d u 2 by d x at x equal to minus b right. So, so these are the boundary condition. Now I have 4 boundary condition 4 here this from these so if I apply on these two then I will get basically 4 equation in terms a b c d and if I; so 4 unknown. So, I will be able to find these value a b c d.

So, I think I will continue in next class.

Thank you for your attention.