Introduction to Quantum Mechanics
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Lecture - 05
Discussion on Bands

In the previous lecture I showed the raising of bands through a simplified version of Kronig-Penny model.

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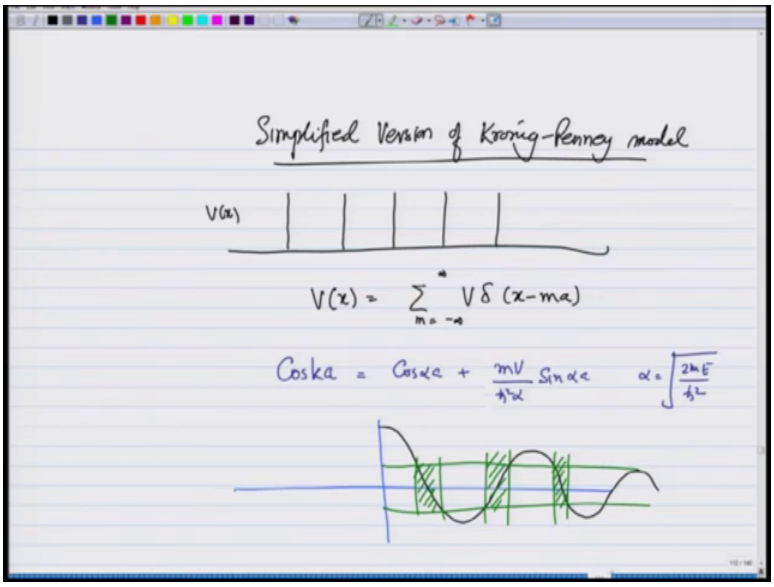

That consisted of periodic potential made up of delta functions. So, v x was given as summation m minus infinity to infinity v delta x minus m a. And what I showed is that if you go through the boundary conditions and blocks theorem you get an equation cosine k a equals cosine of alpha a plus m v over 2 h cross square alpha sin alpha a where alpha is square root of 2 m e over h cross square. And this leads to a picture for the satisfaction of the equation like this and energy is exist because, right hand side should remain below energy bands exist. Because the right hand side should be between minus 1 line one and therefore, energy is exist only in these bands.

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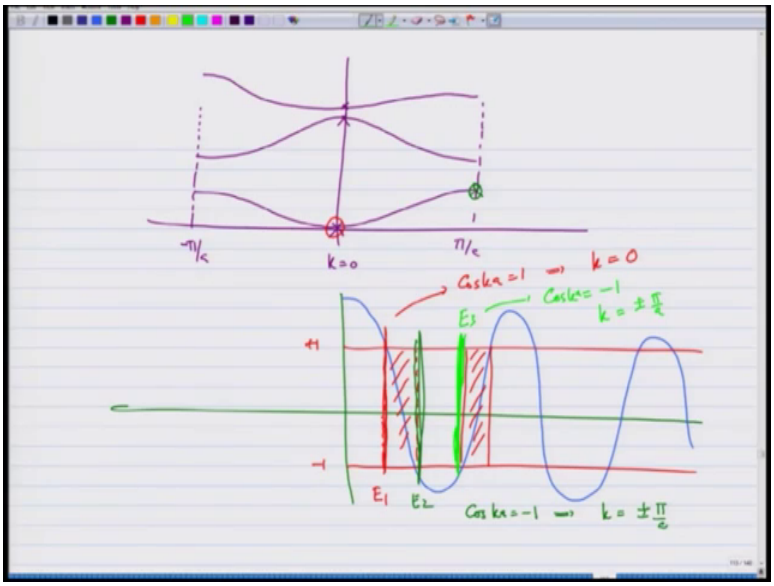

And when we plot it which you will do as a practice where you get these bands are if you restrict between, minus pi by a and pi by a you get energy bands like this and so on. Notice that the minimum exists or maximum exists only at k equals 0 and minima or maxima exists at pi by a, and I left that question for you to think about in the previous lecture let me answer that now.

So, if you look at this curve that we have been drawing the right hand side of the equation looks like this and plus 1 and minus 1 are right here. And energy is in this map notice that where the minimum of the energy first minimum exists right here the by shown by thick red line and I will call it E 1 there cosine of k a is equal to 1 and; that means, k equals 0, if I restrict myself with k b in between minus pi by a and pi by a then the only answer for this is k equals 0.

So, the first minimum exists at 0 which is shown right here. Then the maximum of the energy exists at this E 2 shown by green vertical line E 2. And at E 2 cosine of k a is equal to minus 1. So, this implies k is equal to plus or minus pi by a. And that is why you see this maximum right here shown by green.

Next minimum exists at this bright green line shown here, again by thick bright green line E 3, and that is where cosine k a is again minus 1 and therefore, k is equal to plus or minus pi by a and so on. So, you can see how minimum and maximum of the energy bands exists at k equals 0 or k equals pi by a or minus pi by a.

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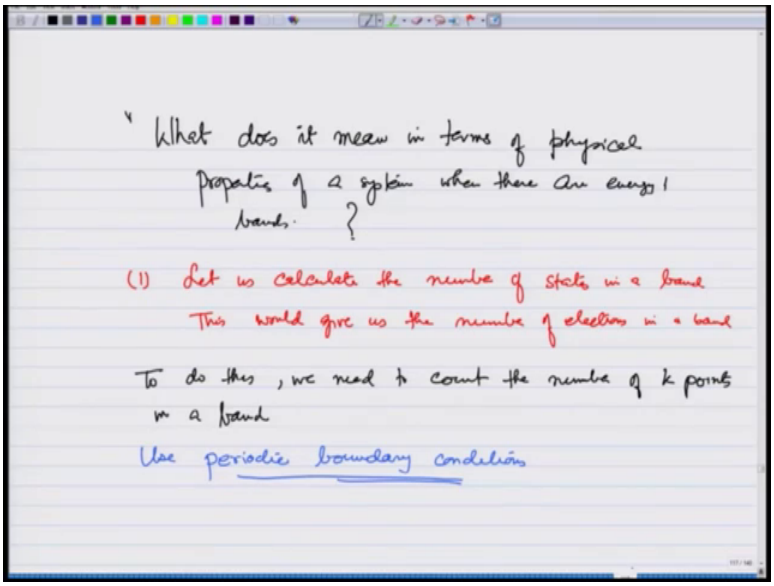

So, in this lecture let us focus on what does it mean in terms of physical properties of a system, when there are energy bands. So, for that first let us calculate the number of states in a band, and this would also give us the number of electrons in a band. To do this we need to count k. So, to do this we need to count the number of k points in a band, just like recall in metals we counted number of states by counting the number of k points. And what trick did we use there, we use periodic boundary conditions. So, use periodic boundary conditions.

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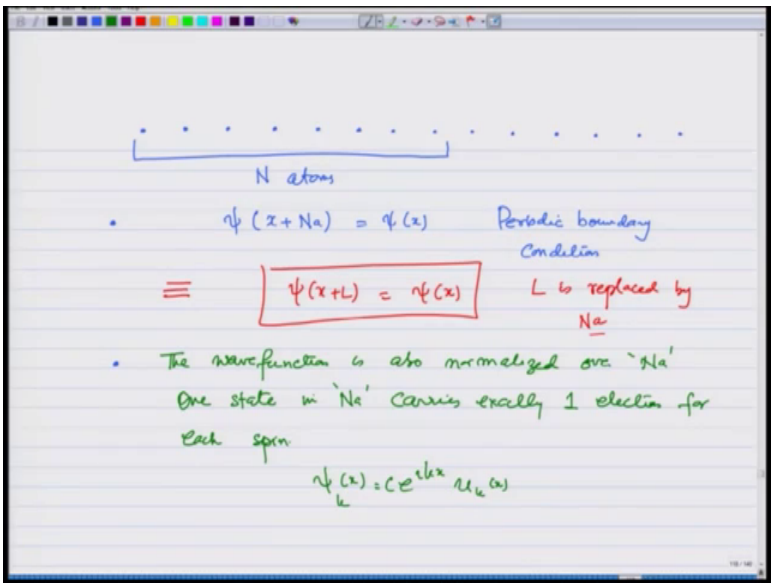

So, suppose we have this set of atoms which are forming a one dimensional metal and this is extending from minus infinity to infinity. What we will do is we will demand that over n atoms, the wave function repeat itself. So, psi x plus N a b equal to psi x. This is the periodic boundary condition. This is equivalent to recall we had in metals psi x plus, l equals psi x this is equivalent to that l is replaced by N a number 1. So, that is point number 1.

Point number 2 the wave function is also normalized over N a, so that a one state in N a carries exactly one electron for each spin. Now to normalize it over N a I can decide to normalize u the wave function psi x recall is e raise to i k x u k x, I can decide to normalize u over entire N a or over a cell and that will just change my normalization coefficient, but that is a material right.

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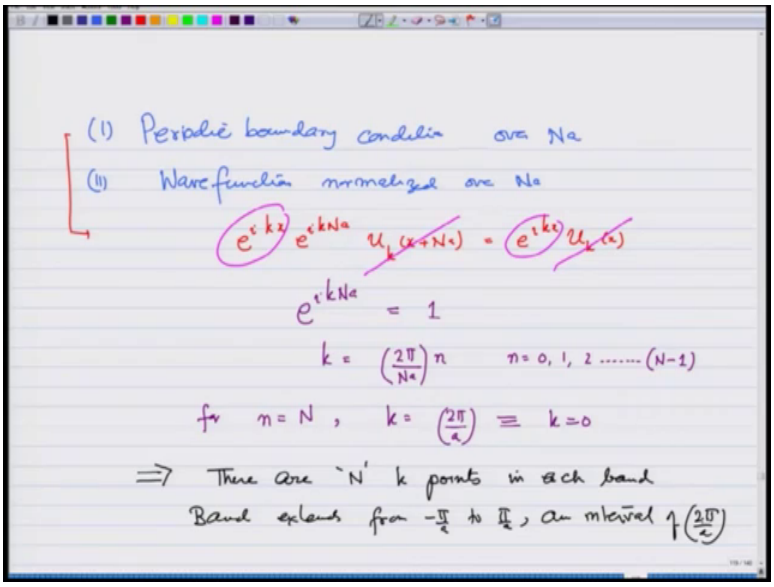

Now so, what the 2 point are making is that one periodic boundary condition over N a and 2 wave function normalized over N a. So, if you do the first point I have e raise to i k x e raise to i k N a times u k x plus N a is equal to e raise to i k x u k x. Now I can cancel u part because u is periodic, I can cancel e raise to i k x part and what I get from the periodic boundary condition is that e raise to i k N a equals 1 and therefore, k equals 2 pi over N a times any number n. N varies from 0 1 2 up to n minus 1. Why n minus 1? Because for n equals n k becomes 2 pi over a, which is equivalent to k equals 0. So, that state does not count. So, what this tells you, that there are n k points in each band right.

Let me repeat it now the band extends from minus pi by a to pi by a. So, that is an interval of 2 pi over a.

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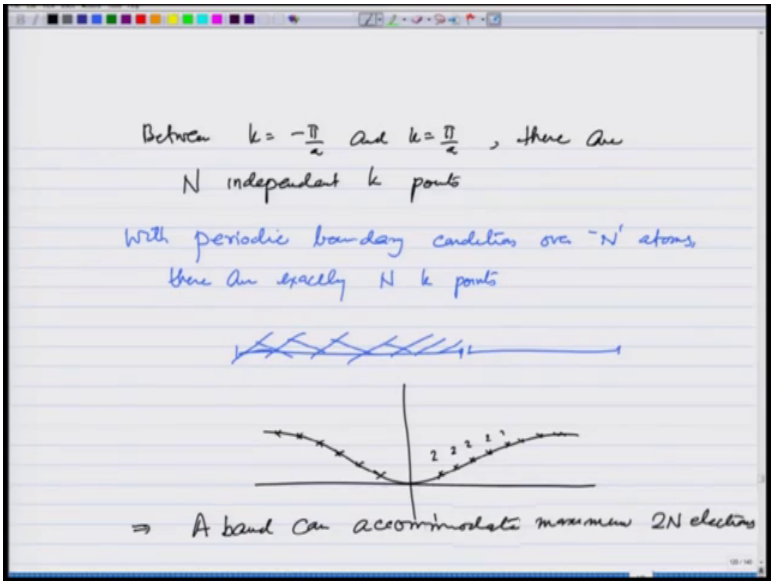

And over 2 pi over a k repeats itself. So, between k equals minus pi by a and k equals pi by a, there are n independent k points. So, with periodic boundary this condition over n atoms, there are exactly N a points all right. My system consists of this periodic thing over n and then it repeats itself. So, I need to focus only on one part here.

So, if I now plot the band, there are these n points. And each of these can carry 2 electrons. So, this means a band can accommodate maximum 2 n electrons.

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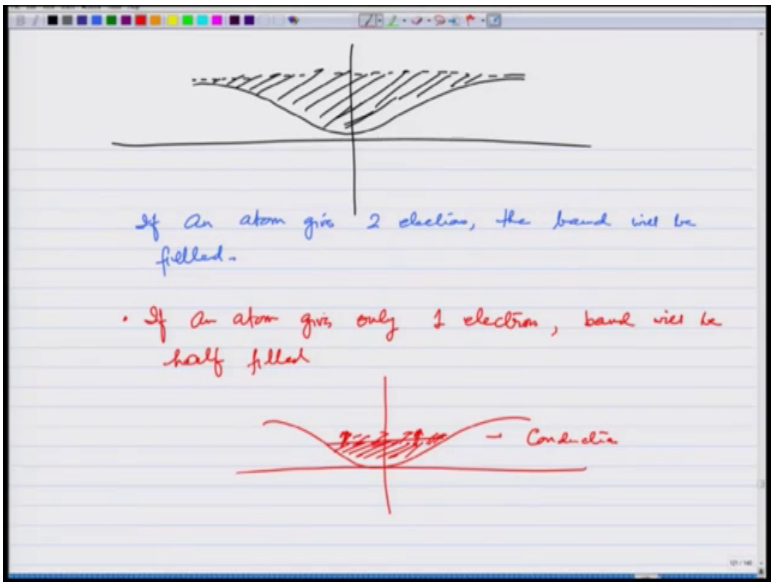

So, suppose I have a band here. The maximum number of electrons can accommodate 2 n and if each atom gives 2 n electrons, this whole band would be filled. If an atom gives 2 electrons the band will be filled.

On the other hand if an atom gives only one electron band will be half filled. Now if I take a half filled band if the band is half filled and I give some energy to these electrons by a pi electric field. They may take energy and go to the higher levels, and that lead to conduction. So, metal is one where band is half filled.

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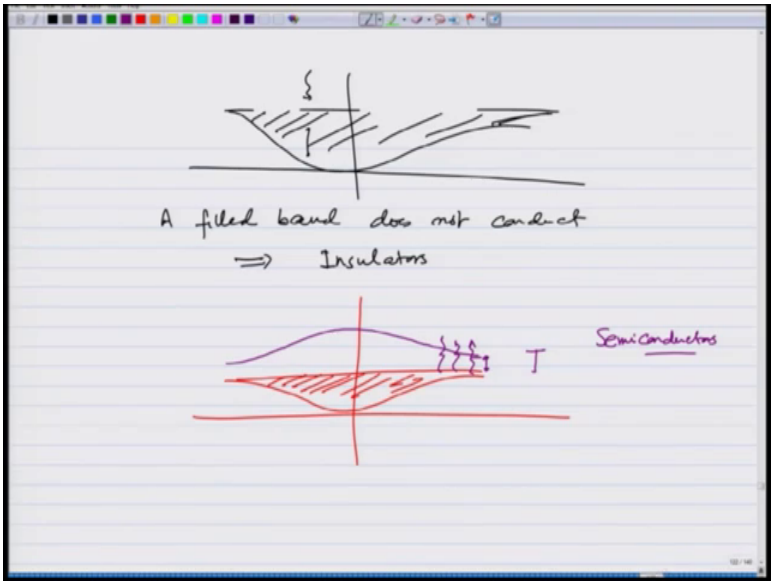

On the other hand if I have a band which is fully filled, if I give energy to these electrons they have no other place to go by Pauli exclusion principal lower energy electron cannot go to the upper energy electron. So, they would not conduct. So, a filled band does not conduct and this gives insulators.

Now, if I have a band which is fully filled, and next band which is close to it band gap is not much, this gap is very small then some electrons can move to the upper band at temperature t. And then the lower band would be less than fully filled upper band would have some electrons and they can conduct when electricity is given, and this gives raise to semiconductors.

So, semiconductors and insulators are both systems where bands are filled at 0 temperature, but in insulators the band gap is very large, and in semiconductors band gap is small. I am giving these arguments for one dimensional systems, now the 3 dimensional has little more certainties, but ideas pretty much the same.

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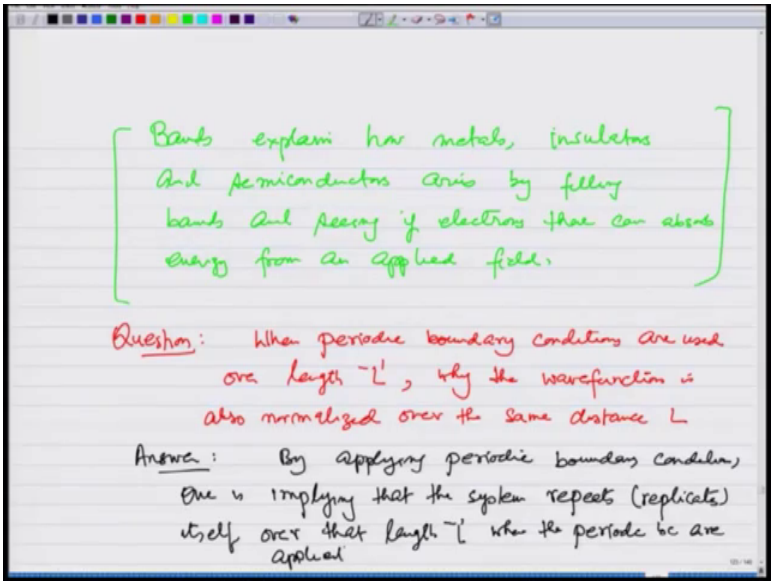

So, bands explain how metals insulators and semiconductors arise by filling bands and seeing if electrons there can absorb energy from an applied field. So, this is the implication of bands that arise in a periodic system. One question that often arises whose answer I am going to give now is when periodic boundary conditions are used over length l, why the wave function is also normalized over same distance l? We did this for metals we did this for semiconductors just now and this question is important because

filling of bands how many electrons can take depends on precisely over what length am I normalize in the wave function.

And the answer is that by applying periodic boundary conditions one is implying that the system repeats or better word is replicates itself over that length l, where the periodic boundary conditions are applied. So, system really is extended over that length l over which I am applying the boundary condition. So, the system is given by that length and then therefore, I normalize all my wave functions in everything over there and that is what gives me the correct number of states n number of k points over for an atoms and 2 n electrons for the same number of atoms.

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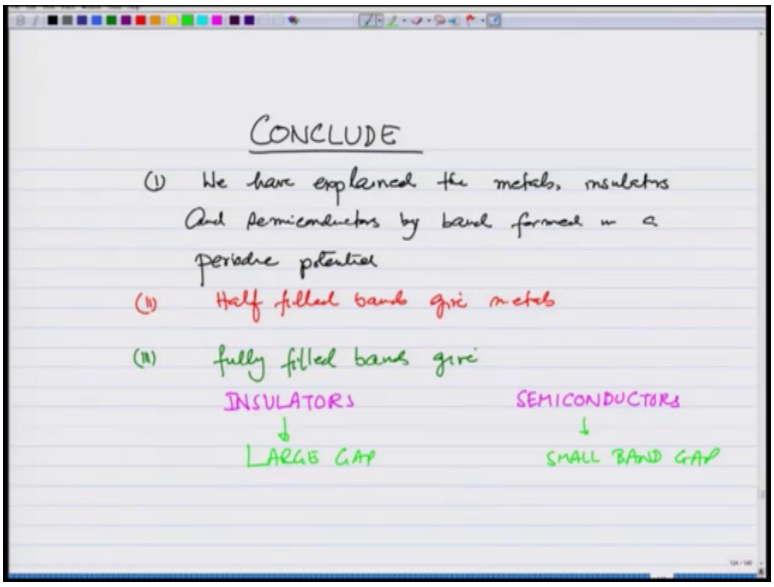

So, to conclude this lecture we have explained the metals, insulators and semiconductors by bands formed in a periodic potential. And what we have said is half filled bands give metals fully filled bands give insulators and semiconductors. This is for large gap, and this is for small band gap.

So, with this we conclude a brief introduction to formation of bands and how they explain semiconductors metals and insulators. So, this concludes our course on quantum mechanics. I will give one more lecture to review the entire course.