Introduction to Solid State Physics
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Lecture – 61
Applying periodic boundary condition to Bloch wavefunctions and counting the number of states

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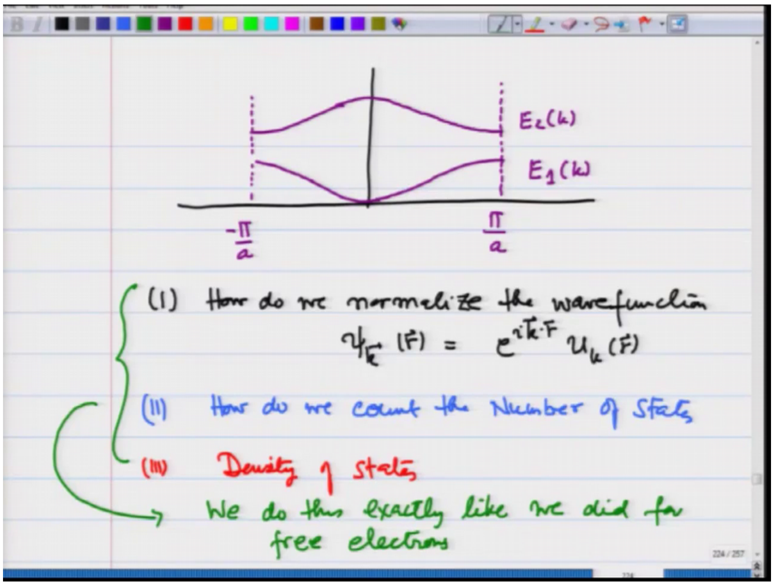

So, far what we have learnt is that when I put electrons are particles in a periodic potential; the energies they can acquire as a function of k form a band of energies, I am making pictures in 1 day and just 2 bands. So, this is E 1 k as a function of energy E 2 k as a function of energy and notice that I have plotted this within the first Brillouin zone and that is to tell you that everything can be specified within the first Brillouin zone only.

Now, we want to count how many states are there in each band and what kind of properties follow by filling these bands as a function of k. So, questions I am raising is how do we normalize the wave function which is the Bloch wave function psi k r equals e raised to i k dot r u k r and how do we count the number of states. And that is important to again find the density of states etcetera which we found that these are quantities which are useful to then calculate the properties of the system.

And answer to all this is only one, we do all this exactly like we did for free electrons everything answered through that we will do exactly same thing as free electrons and this is possible and then we will see its ramifications its impact on how bands are filled and what happens.

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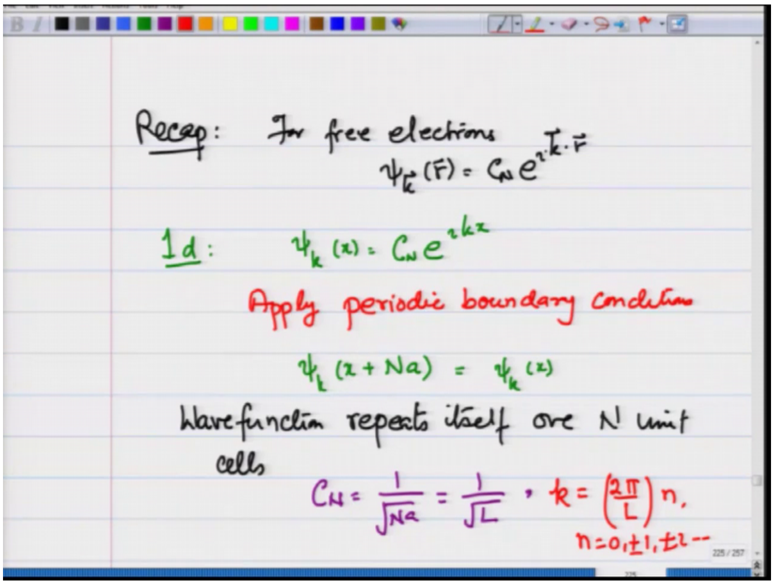

So, just a recap on how we did it for free electrons; for free electrons the wave function psi k r is equal to e raised to i k dot r C N. Again to make life easy, I will do things in 1d the conclusions are the same you will see later differ slightly when in 2 and3d when we look at band diagrams. But right now for1d sufficient so, the free electron wave function psi k x is e raised to i k x and then you put a normalization constant C N in front.

So, what did we do in this case to do all that questions that we raised in the previous slide is apply periodic boundary conditions. And what did that mean? That meant that we said that psi k x plus some Na, where a is the lattice spacing and N is the number of units that we are considering is psi k x.

So, the wave function repeats itself over N units. So, let us write that the wave function repeats itself over N unit cells. And so, it becomes periodic over the n unit cells and that is the periodic boundary condition. And from that we could find that C N comes out to be 1 over square root of N a which is 1 over square root of the length of the crystal or length over which the periodic boundary condition is applied. And k comes out to be quasi continuous 2 pi over a L times n, where n goes from n equals 0 1 plus minus 1 plus minus 2 and so on.

So, this is how we apply the boundary condition for free electrons we do precisely the same thing for block electrons.

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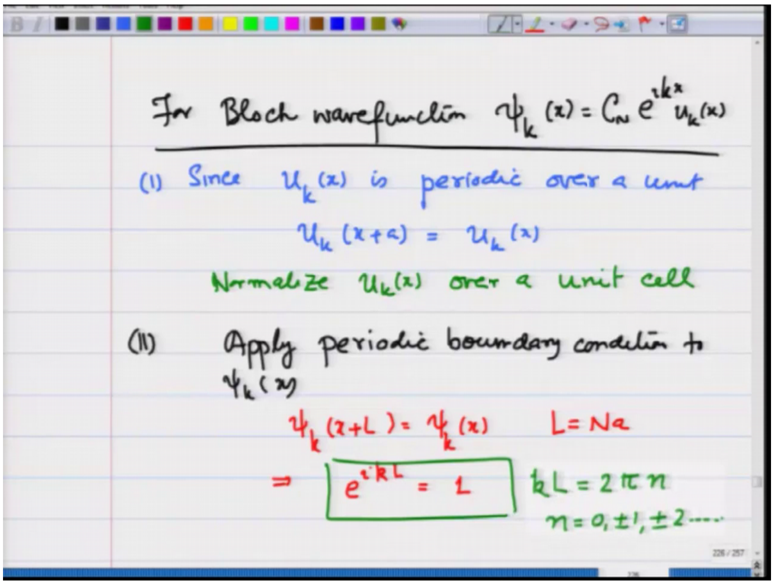

So, for Bloch wave function which is psi k x equals some normalization constant e raised to i k x u k x what do we do? 1 since u k x is periodic over a unit; that means, if i go from 1 unit to the other is exactly the same u k x plus a is same as u k x then we normalize u k x over a unit cell.

So, that part is taken care of and then number 2 apply periodic boundary condition 2 psi k x and what does that mean? That means and then apply the periodic boundary condition over a length L and that means, that psi k x plus L equals psi k x, where L is equal to Na and I am applying these periodic boundary conditions therefore, over N unit cells. Since u k x is periodic over each cell this simply implies that e raised to i k L is equal to 1 that is the result of applying periodic boundary conditions.

I have not shown 1 or 2 steps here because they should be easy for you now taking into consideration that u k x is periodic over each unit cell and this gives k L equals 2 pi n, where n equals 0 plus minus 1, plus minus 2 and so on. So, it gives exactly the same result as in free electron case.

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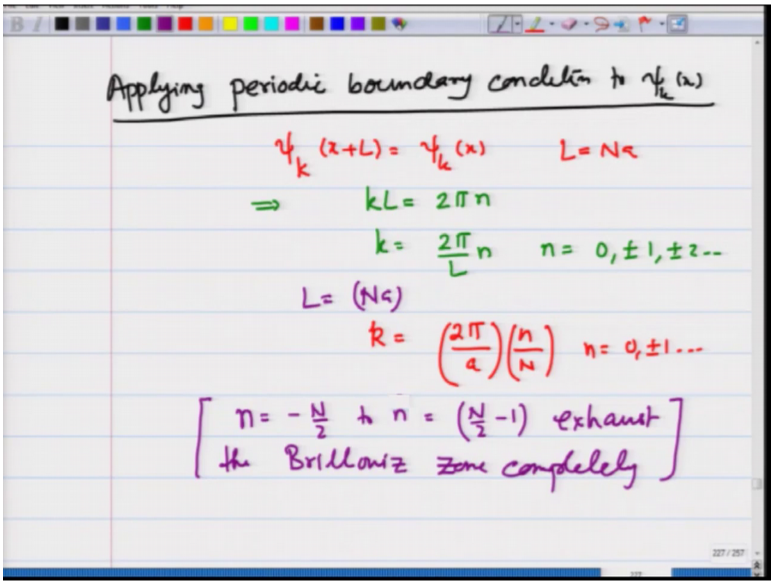

Let me rewrite it. So, what we are doing is we are learning about applying periodic boundary condition to psi k x and in applying this condition I say psi k x plus L equals psi k x L equals Na and that implies that k L is equal to 2 pi over 2 n pi and k equals 2 pi over L n; n equals 0 plus minus 1, plus minus 2 and so on. And since L equals Na i get k equals 2 pi over a n over, n equals 0 plus minus 1 and so on.

And you can see immediately that n equals minus n by 2 to n equals N by 2 minus 1 to be very very precise exhaust the Brillouin zone completely, because you start from minus pi by a and you go all the way up to pi by a minus slight number and then you come to pi by a which is equivalent to minus pi by a right.

So, that part I am saying and I want you to verify it by writing it explicitly on paper. So, when you go from small n to from minus N by 2; that means, you start with k equals minus pi by a and you go all the way up to small n equals N by 2 minus 1; that means, you go all the way up to pi by a minus a very small number because capital N does remember is very large.

So, then you exhaust the complete Brillouin zone and you specify the wavefunction completely by doing. So, and once you do so, what you have done is if I look at this energy versus k curve in the Brillouin zone.

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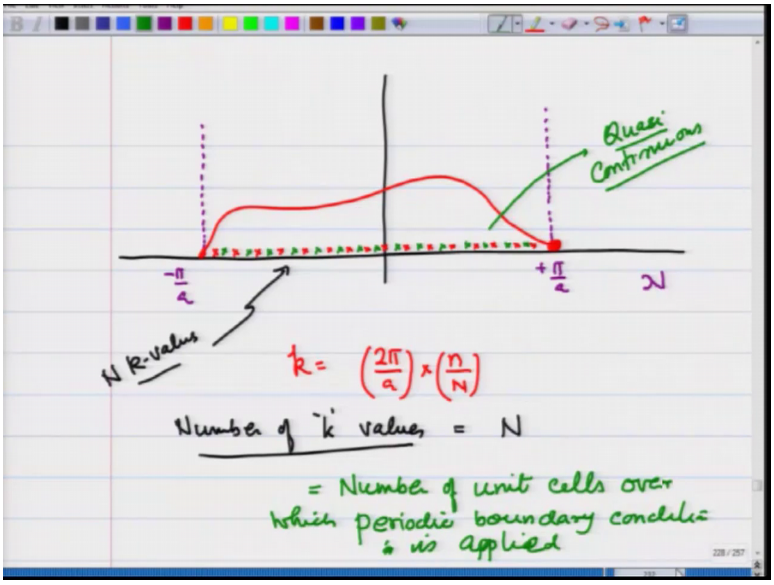

Here is my minus pi by a here is plus pi by a and I have this N says over which the periodic boundary condition is being repeated the k values that I have is 2 pi by a times n over N. So, I have these case if I were to plot are going to be like this I come all the way up to this point and this point the last point is equivalent to this point again.

So, these are the k points that I am going to consider when capital N becomes very very large capital N becomes very large these points start becoming denser and denser and that is what should happen because capital N ideally I will take to be infinitely large I am talking about the entire crystals they will become denser and denser. And these k values therefore, are called quasi; quasi means not precisely like that, but very close to continuous. So, they are not exactly continuous, but very close to continuous.

So, these k values are quasi continuous and the number of k values are going to be N. So, these are N k values all these red and green points i am showing are N k values. So, in a band there you going to have these N k values. So, this is precisely equal to the number of unit cells over which periodic boundary condition is applied.

So, number of k values in a band or number of states in a band is precisely equal to N the number of unit cells over which we are applying the periodic boundary conditions recall that this was precisely the same thing that was there for free electrons as well as the phonon modes. So, when you apply these periodic boundary conditions results are actually quite general they are the same for all sorts of waves. So, N is the number of k values. So, let us see its ramification, so, let me repeat.

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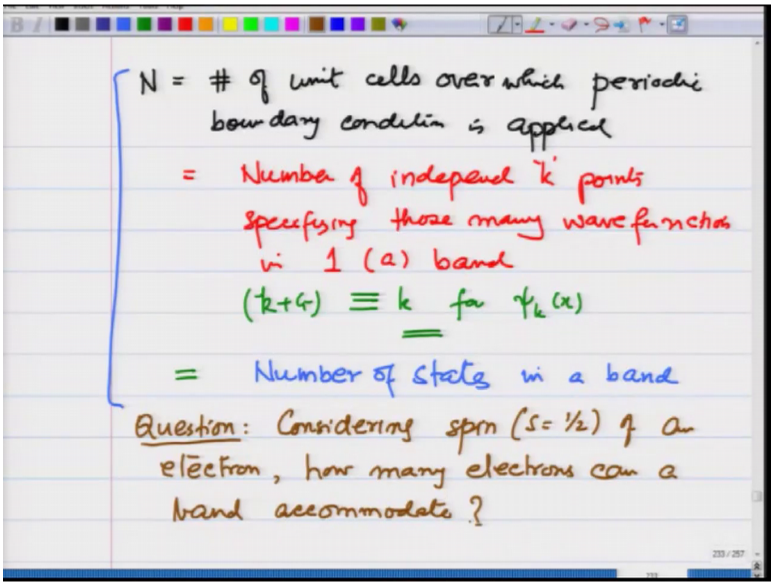

So, N is the number of unit cells over which periodic boundary condition is applied then this is also equal to the number of independent k points specifying then those many wave functions in 1 band right, so, in 1 in a band.

And then you repeat itself and as we have said last time that k plus G is equivalent to k for psi k x and therefore, this whatever you specify within the first Brillouin zone is sufficient. And therefore, number of independent wave functions in a band that we have is N the number of unit cells over which periodic boundary condition is applied. So, this is also equal to the number of states because each wave function gives 1 state number of states in a band.

So, this is what we have learned so far. So, once we have N number of states in a band a question arises and let me write this question now. So, the question that arises is and this is important to now understand the properties of metals semiconductors insulators from band theory point of view the question that arises is considering spin and what is the spin? It is one half of an electron, how many electrons can a band accommodate?

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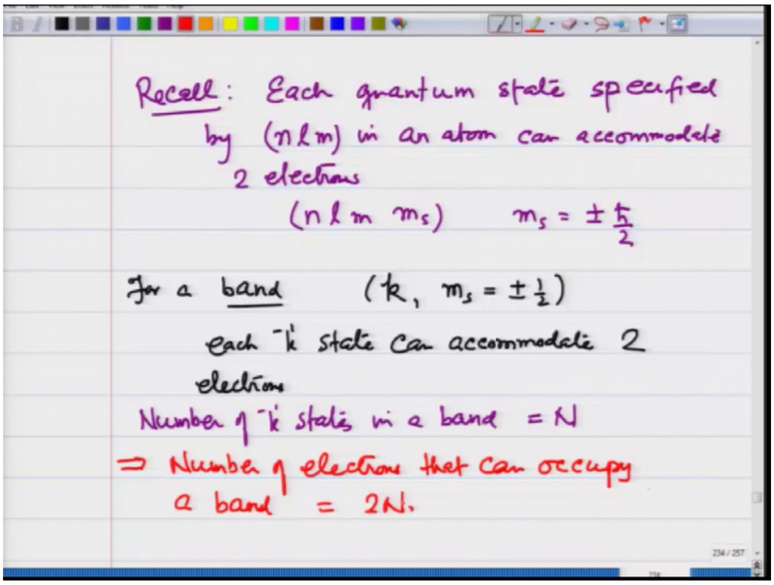

For this I will recall that each quantum state specified by n l m in an atom can accommodate 2 electrons, because each state is now specified by n l m and m s and by Pauli exclusion principle all quantum numbers should be different and therefore, I can have 2 electrons in each n l m state because m s is plus or minus h cross by 2.

Similarly, for a band the crystal quantum number is k. So, ideally if k was the only quantum number it would accommodate 1 electron, but with k I can have one spin up electron and one spin down electron in each k. Therefore, each k state can accommodate 2 electrons and then the number of k states in a band we just saw as N and therefore, number of electrons maximum number of electrons that can occupy a band is going to be equal to 2N.

So, each band now can take 2N electrons, if you fill 2N electrons in a band the next electron will go to the next band. So, let us just show it by a picture.

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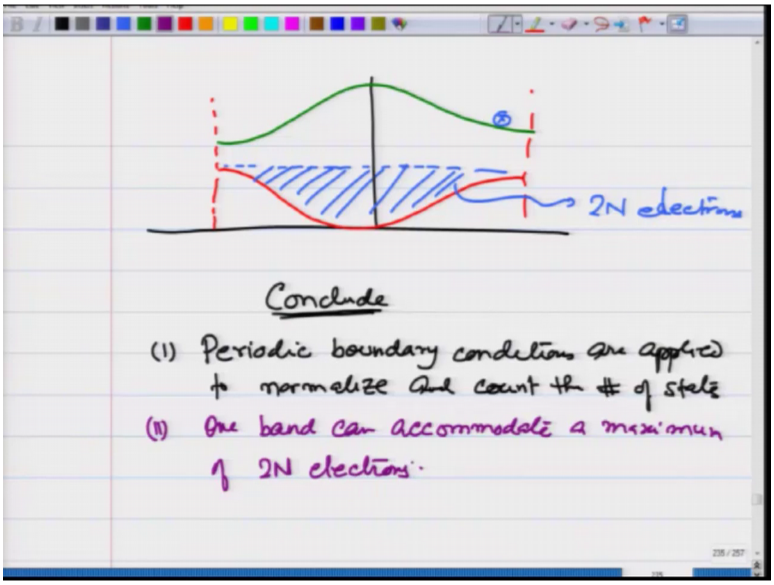

Again in1d I have the 1st band the 2nd band and if I fill the electrons this band can at most accommodate these 2N electrons, we put the next electron we will go to the next band lowest energy.

So, two electrons in one band and this leads to metallic semiconducting and insulating properties of solid this we will discuss in the next lecture. So, let us conclude this lecture by saying that 1 periodic are applied to normalize and count the number of states and 2 one band can accommodate a maximum of 2N electrons.

Thank you.