Electronic Theory of Solids
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Lecture – 13
Bloch's Theorem

Hello. Let us come back to the problem that we were discussing. We want to calculate the bands of a solid, when there are n number of atoms in a solid in a regular periodic arrangement. And we want to basically solve the Schrodinger equation for an electron moving under the potential of all these atoms.

Now, to do that we need to understand a few things before we embark on that solution. And one of the celebrated ideas and theorem that is important to know is the so called Bloch's theorem. And Felix Bloch did it worked it out, and then the theorem basically states about the possible solutions to where to the Schrodinger equation when a particle travels moves in a periodic potential.

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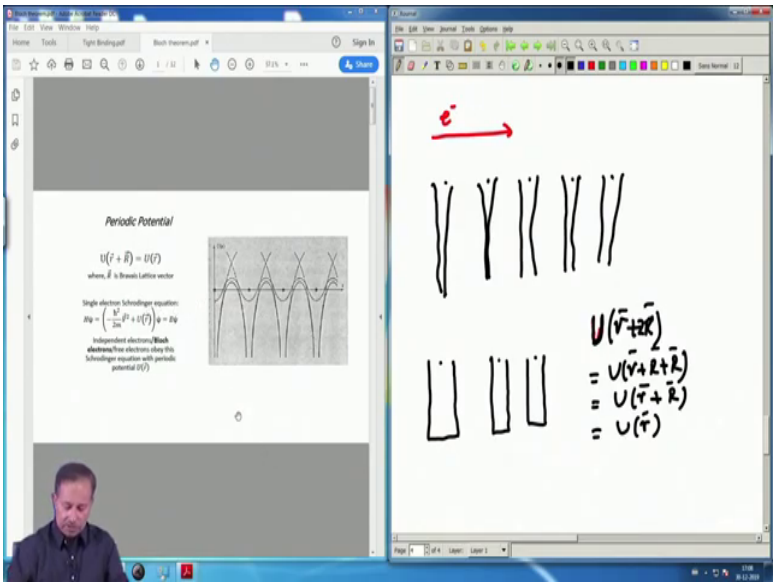

So, let me just first tell you what a periodic potential is, which probably more many of you know already, but let me just digress a bit. Now, a periodic potential is a potential which

repeats which is periodic in space and the left hand picture for example, gives an illustration of such a periodic potential in a one-dimensional lattice.

For example, if I have this kind of a lattice atoms here then the atoms, of course attract the electrons there are potential we will have a structure which is like this; as the electron passes it will see a potential which is like this, right. So, it will be a potential like this, deep potential.

Remember our very 0th level discussion that we replaced these potentials by a infinitely deep potential in a box and that is exactly what we are doing here, but a more realistic just these boxes are replaced by the Coulomb interaction that is they are in a solid.

So, this was the kind of thing that we, kind of picture we drew whereas, now we have fixed atoms, so we are not bringing atoms together they are already there they have fixed distance and in this case we will like to see what and what is the solution of the Schrodinger equation for an electron which is moving in this potential, ok. So, that is the problem.

So, the problem is very well defined. It is a problem of an electron moving in a potential of a periodic arrangement of atoms. These atoms are all having their attractive interaction on the electron and this attraction it has a shape which is what I have just drawn.

On the left hand side, the better drawing has been done the solid black line is the potential it has a deep down at the location of the atom. So, this is the if you can; if you can look at this then if you see this these are the locations of the dots are the locations of the atoms and the potential is deeply positive E square by r and as r goes to 0 it goes a negative minus E square by r because it is an attractive interaction.

So, it goes deeply negative at the location of the potential. As r goes to 0 it will just diverge in the negative direction. But between the atoms of course, it immediately very fast becomes 0 and then the inter atomic space there is a region where the interaction between the nucleus and the electron.

Between the nucleus it has just passed and the nucleus it is coming to this is the both of them are they almost cancel each other and then that means, the electron is more or less free in this region. So, the problem they in mathematical terms is what is written here.

That you have a potential which has this structure. The potential U is such that the potential at any point r if you add capital R to it will just repeat itself. That is exactly the nature of this picture shows that you take the potential at any point r and add this inter atomic spacing a capital R then you will see that the potential is the same at r plus R. So, that is exactly what and you can go on doing it ad infinitum .

So, it is these r can be 1 lattice spacing, 2 lattice spacing, 3 lattice spacing, n number of lattice spacing it will be the same. Actually, these guarantees that right U r plus capital R equal to U r you. So, then you add another capital R then on the right hand side you will get another U r plus R which is again U r.

So, U r; this is the U r plus 2 R for example, 2 into r is U r plus R plus R which is U of r plus R which is again U r. So, you can go on doing this. I mean this is there is. So, that means, n you can add as many capital R's as you want and where you will get the potential to be the same. And capital R here is the in the its basically it is called the Bravais lattice vector which I will come to, but in this one-dimensional picture it is basically the inter atomic distance.

So, the purpose of this whole exercise is to solve the Schrodinger equation under such a potential which is given which is written down here, h psi equal to this is the time independent Schrodinger equation minus h cross square by twice m del square plus U of r of psi is equal to E psi. So, that is the equation that we are after.

So, this is called the independent this is of course. Independent electrons because remember we have only one electron we are considering only one electron or a larger I mean it does not matter if you have n number of electrons which are not interacting with each other.

We will still solve the one electron problem and find out the states, the solutions and put n number of electrons in starting from the lowest solution, lowest eigen energy, eigen state, ok. So, this is the problem at hand, this is what we intend to solve.

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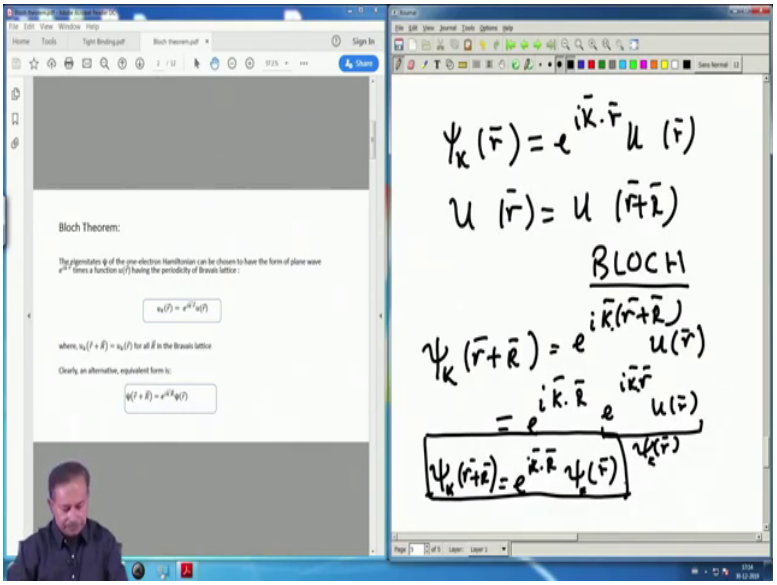

Now, this is where the Bloch's theorem come in extremely handy. Because what a Bloch theorem shows is that the solution, eigen states, let me just state it. The eigen state psi of the one electron Hamiltonian can be chosen to have the form of plane wave e to the power i K dot small r times a function U of r having the periodicity of the Bravais lattice. Again, I will discuss Bravais lattice little bit.

Probably all of you know it, but I will come back to what Bravais lattice. For us for this one-dimensional picture that I showed it is again the inter lattice space. So, this is the, so this psi K of r psi K of r is e to the power i, is like a plane wave except that it is modulated by a function U K of r, but U K of r is such that it is equal to U K r plus R.

So, that is the interesting part to it. So, that is called the Bloch's theorem, Bloch theorem. So, Felix Bloch first wrote it down. In different contexts there is a theorem called Floquet theorem which is similar to it, but let us not discuss that. This is the theorem that is extremely handy and it allows us to choose a certain kind of wave functions.

And it also tells us what should be the property of the wave function that we are looking for the solution. And these an exact theorem, if the periodic if the potential is periodic then your solution must have this form. It is a plane wave, times, a function U of r which is the what I have written down which is which may depend on K, which I may or may not choose K here.

Ideally, it could also depend on K, but hardly matters. We will this for the time being let me not put K here, but this is the general solution. This is the solution that Felix Bloch predicted. This is the nature of the solution. So, this is the property of the solution. It is not that we are giving you a solution we are telling you what the property of the solution should be.

Solutions of course, have to be obtained from the equation, but then we can check whether the solution is follows this theorem, ok. So, alternately you can also write psi K of r is equal to. So, let us just move this wave function by one lattice vector, then let us see what happens. So, e to the power i K r plus capital R in to U of sorry U of r, now r plus R is the same as r, so I can write as U of r, ok.

Now, it is you can see that you e to the power i K dot capital R times e to the power i K r into U of r which is psi of r. So, this is e to the power i K dot r into psi of psi K of r. So, that is a beautiful result because it just tells me that if I move this position of the function by a nearest neighbor lattice side from any side, then I will only have to do is to put a factor i K dot r just a phase factor which is i K dot r where this K will have to be determine that comes from the solution.

So, that we will do later on. But at the moment this just tells me that there is just a phase factor that has to be added to the wave function to go to the next nearest neighbor. To the nearly further one and further one and further one we can just add these phase factors and move on and on and on. So, if we know the solution at a particular r, then we know the solution everywhere, ok.

We know just adding a phase factor we will give me the solution. So, that is a very very powerful theorem. Because you are dealing with an infinitely large lattice and it tells me that if you have the wave function in a particular r then you know everywhere what the wave function should be. So, very very important and useful theorem to work with.

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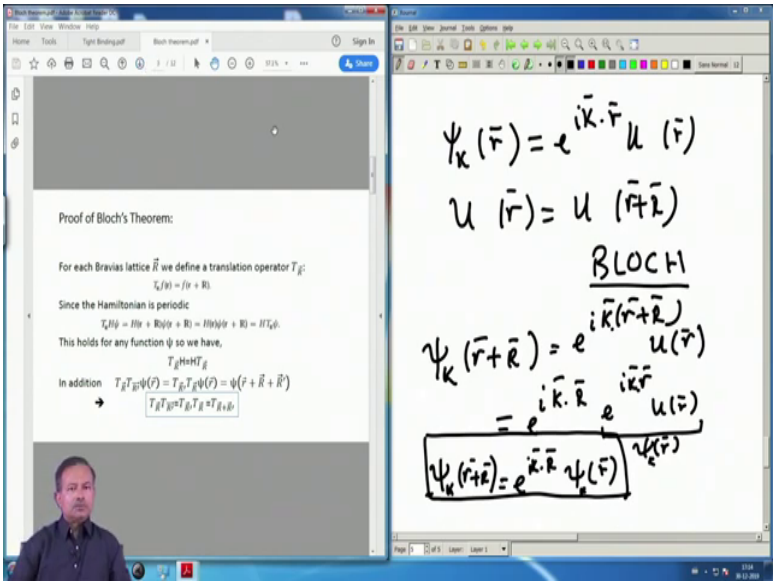

Now, to prove Bloch's theorem let me just go back and discuss a bit about the lattice. We have been talking about lattice, Bravais lattice and so on, so let me just show you an example of Bravais lattice.

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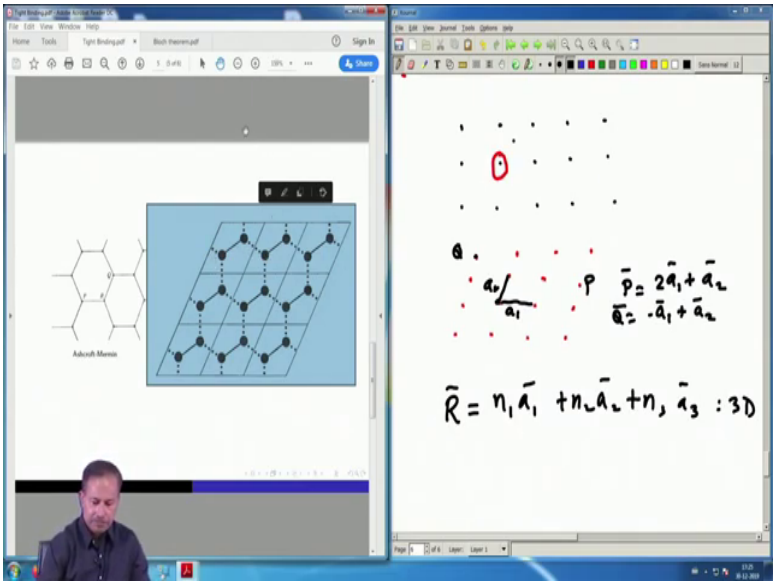

So, take for example, so this is interesting example is a counter example I will just come to what a Bravais lattice is. See Bravais lattice is the definition is very simple. The definition of a Bravais lattice is basically I mean if you have a lattice for example, if you have a

arrangement of atoms for example, this is an arrangement of atom, this is another arrangement of atom.

All these arrangements can be you can see that the in all these arrangements from any point, take any point if you look at the lattice from that point then the lattice looks the same. So, it is not only the arrangement, the orientation will also look the same. So, that is what a there is what is a Bravais lattice.

So, in two-dimension I have drawn now these two lattices both of them are Bravais lattice because from any point you look around you around this point the arrangement as well as the orientation look the same. So, that is called a Bravais lattice. There is a formal way of writing it also, but this. So, let me just write down the formal way.

So, as I said a Bravais lattice is an infinite array of discreet points with an arrangement and orientation that appears exactly the same from whichever of this points the array is viewed, ok. So, let me repeat. It is an infinite array of discrete points with an arrangement and orientation that appears exactly the same from whichever of these points one chooses to look around.

So, that is the way one gives a definition where it is not a mathematical way of looking at it, but it is a perfectly good definition of a Bravais lattice, such lattices, such arrangements are called Bravais lattices. Mathematically you can for example, in three-dimension you can choose a vector. So, say for example, R equal to n 1 a 1 plus n 2 a 2 plus n 3 a 3, where a 1, a 2, a 3 are 3 vectors, not all of them are on the same plane. These in 3D for example, you are doing 3D here.

So, they are in two-dimension of course, they have to in the same plane you do not need the third vector, but in 3D you need this 3 vectors to define it. And these are a 1, a 2 and a 3 are just vectors which any 3 vectors not all are in the same plane and this n 1, n 2 and n 3 are just integers.

By integer 1, means 0 plus integer minus in negative integer all. So, this is basically the definition of a Bravais lattice. So, these R, capital R spans a or generates a Bravais lattice. So, that is the formal another way of looking at it. It is a mathematical way of writing it down.

These vectors a 1, a 2 and a 3 are called the primitive lattice vectors and they generate these the Bravais lattice a by generating these points R, every point R by generating from n 1, n 2, n 3 being integers you can just generate as many R s as you want and that generates the Bravais lattice.

So, as I give an a example. For example, this is this in this case for example, I can choose two vectors a 1 and a 2 and this is my origin. So, take the point for example, this point P and this point Q. I can write P as a 2 a 1 plus a 2, right. The vector P connecting origin to P can be written as 2 a 1 plus a 2.

So, these n 1 here is 2, n 2 here is 1 and n 3 equal to 0. Similarly, if I want to get to this point Q then I will go my minus Q will be minus a 1, so I come here and then go one step a 2. So, minus 1 and 1 at the and 1 and n 2 here. So, that is exactly what one is saying that this definition of this Rs that you can generate are making giving you the lattice that you want this is that lattice is called the Bravais lattice.

Now, here is on the left side I have chosen a I have shown a chosen to show actually a Bravais lattice which is not a Bravais lattice. Now, let us look at this left hand side picture this one for example. Now, if you look at this lattice look at the point P and then look at the point R from P if you look around the arrangement looks to be the same, but the orientation is not just look at carefully from the point P which is this point, this point P, this.

So, this point has a point on the left side right on here, if you look up left there is a point here nearest neighbor whereas, these R does not have a point here. So, that is an interesting example that this lattice is not a Bravais lattice. In fact, you can actually check for yourself if you take this a point P and R, if you take point P the neighborhood that you see will be seen exactly from the point R if we just rotate this page 180 degree.

Just from just rotate 180 degree half circle then you will see the this, so you rotate it by 180 degree this picture then you will see that Q, R will now look like P, the neighborhood of R is exactly like that of P. So, this is interesting exercise you can take a print out of this or just draw it on a P piece of paper and rotate it and see that the only if you rotate 180 degree can

you can your P and R look the same. By looking the same I means view the lattice from that point and your view should be the same.

So, for example, if you look at Q, Q is very similar to P exactly similar to P actually the view from a Q and a view from P are the same. And this lattice is actually a honeycomb lattice and this is not a Bravais lattice, although this is a lattice. This is a regular, I mean by lattice I mean a regular arrangement of points, but its orientation has this problem that it is not the same viewed from every side. So, that is not a Bravais lattice.

Now, so the interesting thing you can also check is that if you put a pointed the middle of this lattice another point in the every new every hexagon you put one middle at the middle another point you will end up getting a triangular lattice and that is again Bravais lattice again.

Then, you will find that all points all points represent same view whichever way you look at. So, this is a celebrated example now because for the last 10 or 15 years graphene is the hot topic, everybody discusses a graphene. So, many new properties have come up for graphene and you can look up in the literature and see that graphene has these kind of a lattice.

So, the question then is what does one do with that kind of lattice. Can't one do a band structure for this kind of a lattice? The answer is of course, yes. You way to do is do it is to choose a unit cell which will for example, which when you after you take the you make the unit cell choice every unit cell should become equivalent.

So, that is a choice has been shown here. For example, each of these parallelograms here on the right hand side, each of these parallelograms that you have has two atoms of this lattice, assuming that the atoms are all the same. Both the, both atoms are same or even if they are different you could choose, but these in graphene for example, both are carbon atoms.

So, then what you do is that you choose your unit cell to be this parallelogram for example, and any point inside the parallelogram can be chosen as a new lattice point. And the equivalent point in the next parallelogram has to be check chosen as the lattice point and that way you can construct a new lattice and that lattice is a Bravais lattice.

So, this is called the choice of unit cell and the unit cell with a basis. So, this for example, in this case when I had this choice on the right hand side for example here, this I could choose the unit cell with only one atom because all atoms are equivalent, viewed from, view if you view the lattice from every atom it is equivalent.

But here it is not, so I have to choose a unit cell in such a way that if you again becomes equivalent and then of course, this is a Bravais lattice of the new lattice. With lattice with a basis is again a Bravais lattice on which we can now do a band structure. That is more complicated, but it is doable and it is routinely done.

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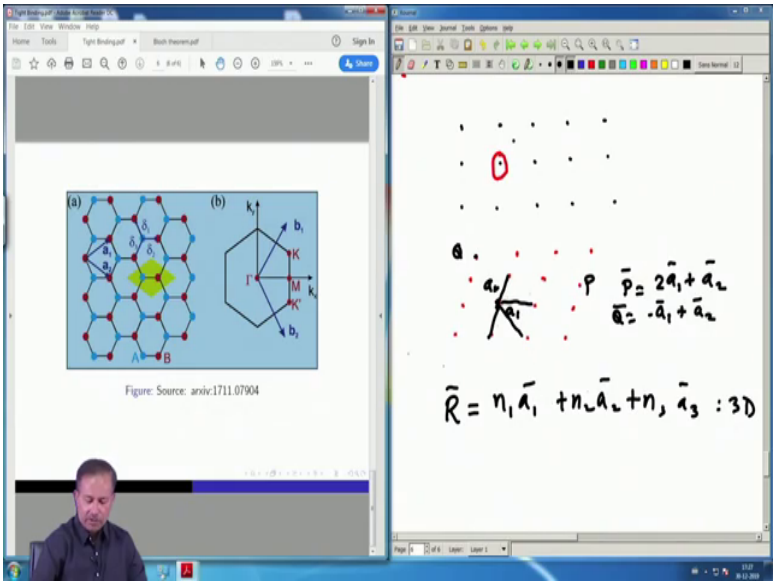

So, this is for example, the celebrated example of graphene. So, what one shows here is a and b are the, a is the real lattice and b is the reciprocal lattice. You have all done reciprocal lattice. So, the reciprocal lattice is constructed here. Reciprocal lattice of this kind of a lattice is a hexagon and so it is you it is just a rotated hexagon you can see that the line here is at the top, here the point is at the top, but it is still a hexagon.

And the other thing is that you can choose these vectors a 1 and a 2. This choice is not unique remember, I could for example, on the right hand side this picture I am showing I could as well choose any two other vectors. For example, I could choose this and this as my new unit vector, new a primitive lattice vectors. So, that will perfectly describe the lattice again. Every

point can be described by that lattice choice, this choice of unit cells, choice of a primitive lattice vectors.

Here a convenient choice is for example, a 1 and a 2. So, these a 1 and a 2 represent the a 1, a 2 that I have written here and lattice is spanned by this these two vectors. And the unit cell that you have to choose is this yellow one, which is what I have done in the previous slide for example, and the Brillouin zone is this a right hand side b, gamma point is the central point K equal to 0, 0 0.

This is called M point, this is K point and this is K prime point, these two points are in equivalent and so and then the reciprocal lattice vectors are b 1 and b 2. So, this is how graphene is worked out. And at some point if we have time I just tell you what the band structure of graphene is because that is very important in today's context.