Electronic Theory of Solids
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Lecture - 18
Fermi Surfaces

Hello, we have been studying the consequences of an electron moving in a periodic potential. And we used the theorem called Bloch theorem to show that the wave function should have a particular form; that it is if you translate by a Bravais lattice vector the wave function picks up only a phase which is e to the power i k dot r where, r is that Bravais lattice vector.

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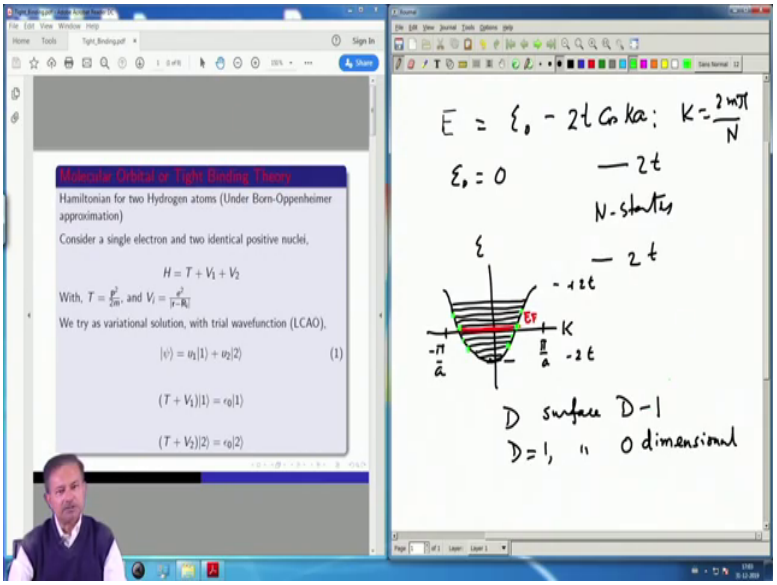

So, this led us to the formation of bands. For example, the band formation means that you have in 1 dimension for example, your energy is epsilon 0 minus twice t cosine sum k times. If I put the a explicitly the lattice constant then it will be k a; where k a takes some discrete values depending on the periodic boundary condition or open boundary condition that you use.

So, for example, k in one case is sum 2 m pi by N and so on. So, that is the solution that we actually we wrote down. So, the band then suppose I said epsilon equal to 0; then this band goes from minus plus 2 t to minus 2 t with N states in between; each state can take care of

two electrons. So, can accommodate two electrons and; that means, that if you are at half filling, then your Fermi surface will be at a Fermi level will be at the middle of the band.

So, for example, this kind of a band will look like from minus pi by a 2 pi by a this will be like this. So, this will be minus 2 t this level will be minus 2 t and this will be at plus 2 t ok. So, that is the solution and you have to put in a large number of N number of energy levels in between and so on.

Now, you depending on your filling, suppose you are a half field so, you will only fill up a half the number of states and your Fermi level will be somewhere here EF. Now, remember this is a E versus K graph. So, this is E versus K graph and this is 1 dimension and this one has a Fermi level is at EF.

So, where is the Fermi surface? Now in any dimension D a surface has a dimension D minus 1 ok. So, in 2 in 1 dimension the surface will be basically 0 dimensional. So, D equal to 1 the surface is a 0 dimension ok. So, this 0 dimension surface means its basically a point and you can identify those two points those two points are these points this point and this point.

So, these are the so, called Fermi surfaces or Fermi points in a 1 dimensional tight binding model for half filling. As you increase the filling the point will move up it might come here it might come here. Or if you are reducing the number of electrons you are going to lower fillings then it will be somewhere here or and here and here and here.

So, there will always be these two points where the constant energy line which is a line here which is a surface in here in D dimension any D more than. So, this is a so, this constant energy surface so, called constant energy surface is a set of 2 points in this D equal to 1 dimensional problem any finite dimension of course, D equal to 2 that will be aligned D equal to 3 that will be a surface as we know it 2 dimensional surface and so on.

So, let me just illustrate this again with a by showing the Fermi surface for example, in a case which is a very well known. And for example, the 2 dimensional; so, let me just show you the Fermi surface in the 2 dimensional case this is what we have been doing.

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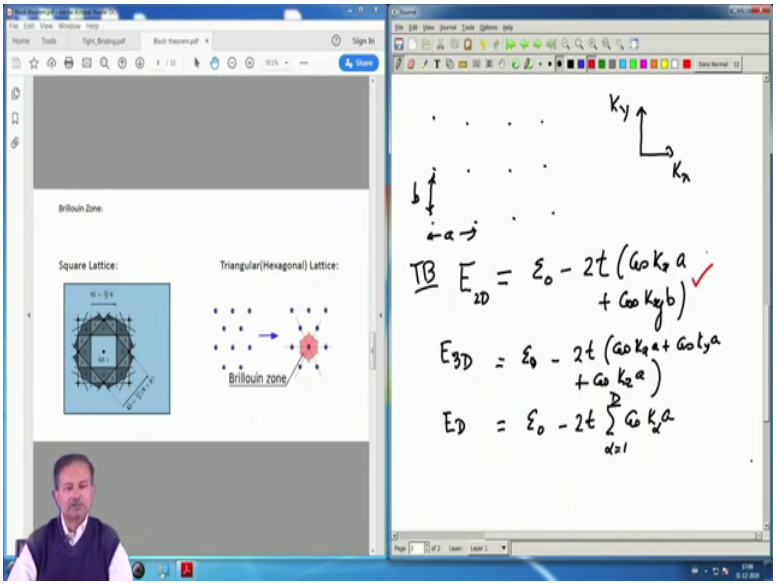

So, this is for example, is the Brillouin zone for a square lattice this left hand side. Now, this Brillouin zone basically implies that my states that I will calculate we will fill it in. So, let us just let me see show you what a 2 dimensional energy spectrum will look like in tight binding model; its very straight forward actually knowing the 1 dimensional.

Suppose you have a square so, a square is an ideal example where the two directions are orthogonal to each other. So, if you draw a reciprocal lattice that will also be a square. So, then there will be a k x and k y; these are orthogonal. And the spectrum; that means, these spectrum will just be set of 1 dimensional spectrum in each dimension.

So, what does that mean it means E as a function of k is again some epsilon naught minus 2 t cosine k x into a plus cosine k x k y into a. Now of course, I could the choose a or and b as two different lattice constants in the two directions, that would be just that would just make this just a b.

Then if you had a in this direction lattice constant a in this direction and b in this direction sorry b in this direction then there will be a cos k x into a plus cos k y into b in a square lattice of course, a equal to b. So, that is why I wrote k x a plus cos k y b. So in 3 dimension for example, this will be just epsilon. So, this will be E 2 D in tight binding nearest neighbor tight binding.

So, in 3 D it will be similarly E some E 0 minus twice t cosine k x a plus cosine k y say this is a all lattice constants in all directions are the same. So, k y a plus cos k z a otherwise I will write a b and c if the lattice constants are different this is for a cubic lattice. For any D dimensional lattice, D dimensional lattice of this kind this is called the hyper cubic lattice you can generalize these lattice a square to cube to a cube in any dimension in D dimension.

So, that will be like minus twice t basic sum over alpha cosine k x k alpha into a if all the dimensions are the same lattice constants along all the dimensions are same. So, these alpha will go from 1 to the number of dimensions. So, that is the spectrum. So, its actually very straightforward for cubic lattice to do it.

For one triangular lattice or FCC or BCC that kind of lattices is more complicated, but it is still durable all you will have will be there will be a cross terms between k x k y and so on. Cos k x into cos k y kind of terms will appear with suitable form factors like root 3 by 2 in for triangular lattice and so on.

So, that is a just a technical detail, but for a square and cubic or even 1 dimensional lattice this is absolutely straight forward. And what I am writing down is just a generalization of the 1 dimensional problem into 2 3 and higher dimension for hyper cubic lattices. So, now let us just concentrate on the on 2 dimension this one the 2 dimension. Now I have of course, a k x k y surface so; that means, I my plot e versus k will be a 2 dimensional plot ok.

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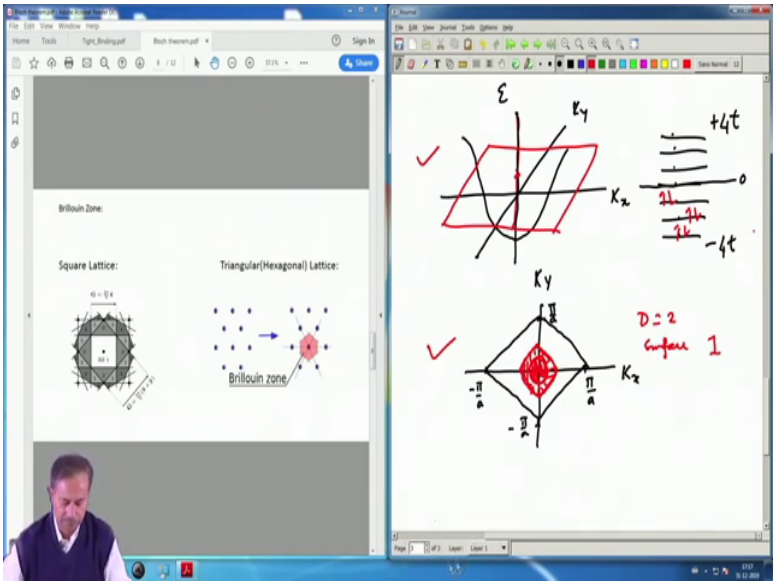

So, let me draw it with black its a 2 dimensional plot. So, this is k x this is k y and this is epsilon e energy and epsilon naught I again take to be 0. So, in that case you can easily see that this will be like a bell, but now in 2 dimension its a 2 dimensional surface. So, it is its like 1 dimensional surface is rotated like a bell along the this z axis.

So, then of course, if I draw a constant surface here which is for example so, this is a constant surface if I draw is a surface of constant energy; because it intercepts this axis at a particular point energy axis and its horizontal. So, this energy surface cuts this bell kind of structure inverted bell kind of structure at points which are along the surface of it.

So, then of course, for tight binding model we can determine exactly how that surface looks like. So, that is what one let me just show you here for example, this is the first Brillouin zone. So let us just write as I said that I can reduce everything into the first Brillouin zone. So, my band structure basically is I will draw only in the first Brillouin zone. And the example that I have given I have only one orbital.

So, I will be; I will be living in the first Brillouin zone only. So, let us just plot the. So, this is a k x k y now of course, you have pi by a minus pi by a and then you have plus pi by a along a y direction and minus pi by a along k y direction as well. And you if you look at your Brillouin zone this is your Brillouin zone.

So, now you have to fill up this Brillouin zone that depending on the number of electrons you will basically fill and you will find for example, if you have a very low filling then your then your Fermi surface will look like a circle around this gamma point this point is the gamma point central point; as you increase you start filling up the Brillouin zone and so, that is how the Fermi surface will look like even it will become a more like this as you increase the filling and so on.

So, that surface that red surface is the region that is filled up filled in is this. These are the states which are filled out if you increase the chemical potential. If you increase the filling the number of electrons, density of electrons then it will increase to this one and so on and so forth it just keeps on increasing.

So, that is how the Fermi surface is plotted. So, I will let some point show you some band structure and some Fermi surfaces that are a for real materials of course, in 3 dimensional real materials its much more complicated, but we will demonstrate some of this. But for the time being let me ask you to at least do it yourself for the 1 dimensional case find out the 2 Fermi points; here it will be Fermi lines remember these are this is just a line, the so called outer surface the surface is a line here.

So, D equal to 2 so, the surface has a dimension 1. So, this is the; this is the line that I am talking about; this is for lower filling the line is almost like circle the periphery of a circle the inner region of that is filled up. So, that is the highest occupied energy surface in the D dimensional plane, which is D which has the dimension of D minus 1 the surface has the dimension in D minus 1 ok

So, this is how Fermi surfaces are drawn and this is how the band structure once you do the band structure then the procedure is very simple; once you do the band structure calculation you have this set of energy levels.

For example in 2 dimension it goes from minus 4 t to plus 4 t; you can check it see in 1 dimension it goes for from minus 2 t to plus t in 2 dimension there is another cos k added to it. So, it will go from minus 4 t to plus 4 t and then c epsilon equal to epsilon naught is 0 still assumed here. So, my 0 is somewhere here.

So, around 0 to be symmetric if epsilon naught is if you want to insist on taking epsilon naught you have to just shift this band structure that much above or below depending on epsilon naught is positive or negative. Now the point that I am trying to make is that the prescription is now very simple; these are the one electron levels and you suppose you have N number of electrons. So, you start filling up from the bottom and go ahead do it 2 electrons per state and go ahead and do it.

And then you will find the highest occupied energy level is your Fermi level there is the Fermi level. Let us call Fermi level there is an energy and the if you cut your band structure the this one for example, at that energy then you will find the surface. So, that is the surface in here which is a line that surface is a line in this figure. For example, in the bottom figure it just is this line outer line of the red part the bounding line.

So, of the field part of the Brillouin zone. So, that is how one actually does its very simple the prescription is extremely simple and this is how band structure and band filling and Fermi surface determination are always done. Of course, there are experiments which are very powerful experiments which do the band structure which not only can find out the band structure.

Particularly in nearly Fermi surface, it near the Fermi level and there are also methods which employ a strong magnetic field at low temperatures to find out the Fermi surface. So, those are methods that are experimental methods to determine the Fermi surface of a material. If you can look up any solid state physics book, then you will find these methods are described and they are very powerful methods to describe a to find out the Fermi level and the energy bands close to Fermi level and the Fermi surface.

The interesting thing is that the for an insulator of course, there is no Fermi surface because there is a gap. So, the highest occupied level in an intrinsic semiconductor for example, will be at the midway of the gap. So, there are no states there. So, there is no Fermi surface to talk about ok. So let me show you some band structure real band structures which are.

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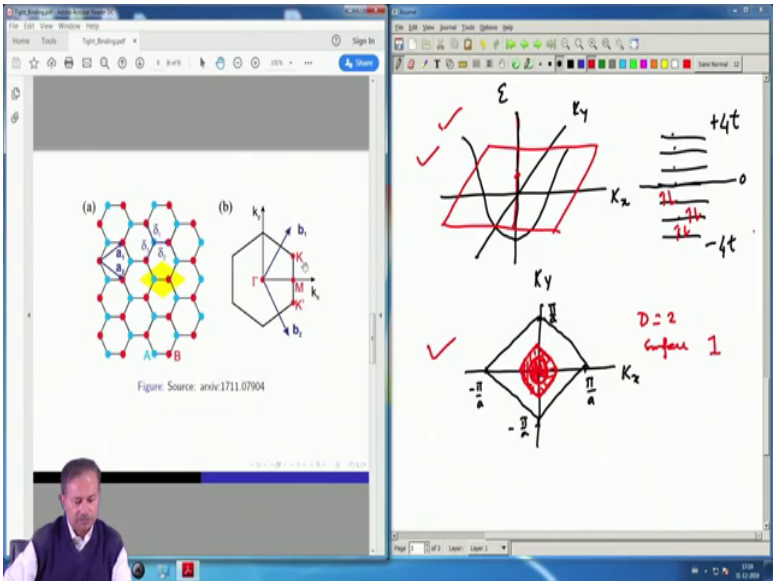

Here for example, this is for as I said for graphene; the band structure requires you to go to a lattice with a basis. So, they are the band structure is fairly interesting.

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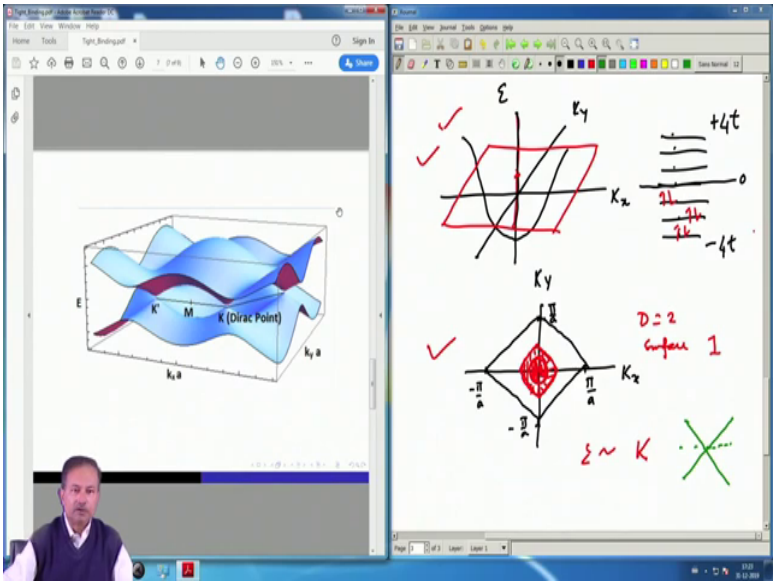

And its complicated in the sense that look at the 3 dimensional figure. This is again you can see this is same figure that I have drawn on the right hand side here its not identical, but it is the same principle that one has used k x and on one axis k y on the other axis. And so this is k x axis this is k y axis and then energies along this third direction z direction. And remember, I

mentioned that there are symmetry there are directions here along which one generally plots the band structure.

So, there the gamma is the central point k x equal to k y equal to 0 and there are this special points symmetry points called K a K prime and M and look at the band structure. K at K and K prime the upper band and there are 2 bands because there are remember the unit cell has 2 atoms and these atoms are inequivalent; although they are both carbon, but they are in equivalent in the sense that the view of the lattice as I say from these two are different. So, they are not equivalent in terms of a symmetry.

So, there will be 2 bands; there will be twice the number of bands as we twice the number of states as we did in this our example. So; that means, if we had only single atom in the unit cell we would have some N number of states coming from the N number of sites if only one orbital was considered per site. Now you even if you consider one orbital per site for these two inequivalent sites will give two orbitals per unit cell and that will lead to two N number of states.

So, two different bands will now appear and so that is what is being shown here the close to Fermi level this is what happens that. There are these two bands and these bands touch at this point K prime and K and these are as written these are called Dirac points and this has a significance.

Because if you remember quantum mechanics then and relativity of course, then you know that in a relativistic physics the spectrum e goes as K not K square. So, that means, the this the and the equation in quantum mechanics that governs these relativistic particles; its called the Dirac equation as it is just the counterpart of Schrodinger equation which is the non relativistic equation for the for quantum mechanical particles.

So, for relativistic cases, the state the corresponding equation being Dirac equation one finds a spectrum which is linear in K. And if you have a linear in K spectrum that is called a Dirac spectrum and these are the two points K and K; K and K prime where one actually finds a linear spectrum. So, that is where the bands will in the in graphene the bands will be like this like v kind of structure.

So, two bands are meeting here as at a. So, these this spectrum as you can see is like a V. So, let me just draw it again it will be simply a V kind of structure and this is the Fermi level. So, that is exactly what is being drawn here, but look at the band structure at M point there is a gap.

So, this is the graphene band structure is rather strange; because you have a Dirac like spectrum at two points in the Brillouin zone and you have a gap at this M point in the Brillouin zone. Remember this points K and K prime are here and M is in the middle.

So, their band structure is has some peculiarity, which is which extremely important for the myriads of strange properties that graphene has shown so far. So, its a single sheet of graphite and its a honeycomb lattice with only carbon but the spectrum has led to such beautiful interesting physics; that we will that I am basically tempted to show you the spectrum. So, let me just show you one more.

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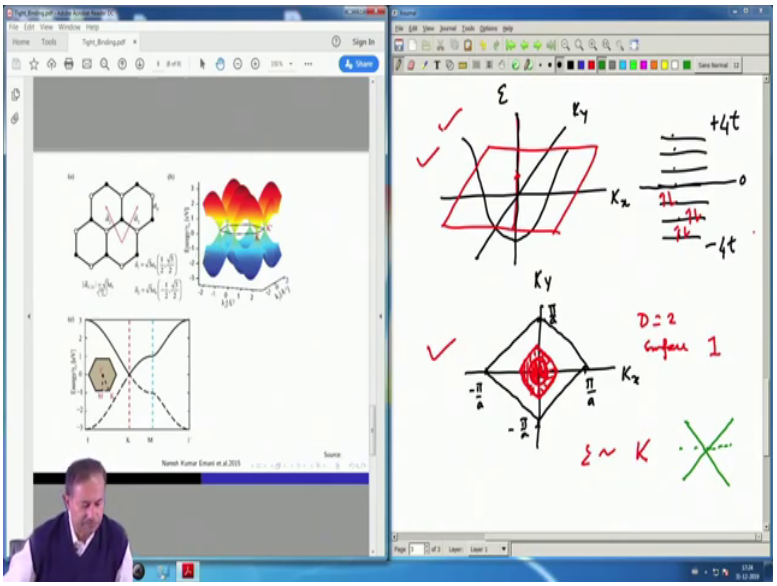

So, this is how the this was shown to you already the left hand top corner; this picture is already there up the a 1 and a 2 are written down here their coordinates are given the vectors are given. These are the two unit vectors in the real lattice; you can as I said you can choose your primitive lattice vectors in any way you want.

So, then this is the spectrum this is the; this is the band structure that you will obtain the lower curve this one ok. So, again the you remember this points the gamma M and K. So, generally, the band structure is plotted along certain symmetry direction which I will just come to in my next lecture.