Electronic Theory of Solids
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Lecture – 22
Fermi Surfaces Instabilities

So, we have been; we have been working on these tight binding approximation for certain lattices.

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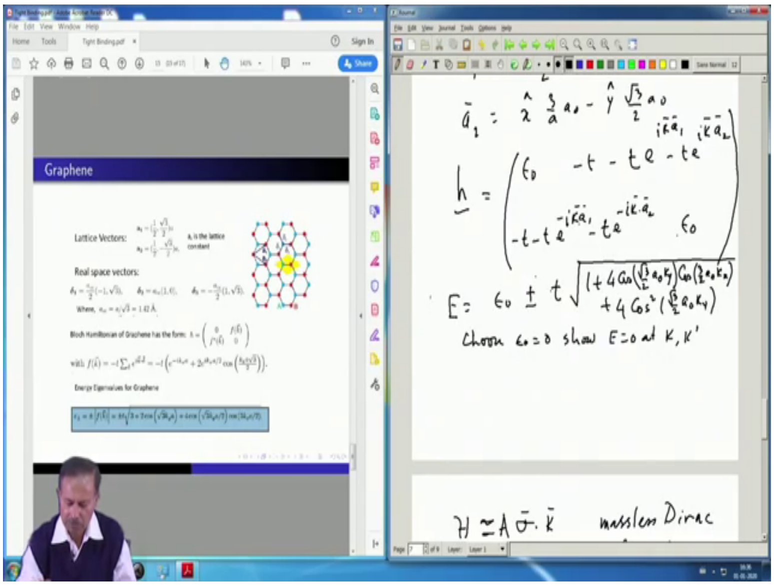

Graphene

Lattice Vectors:

Real space vectors:

Bloch Hamiltonian of Graphene has the form:

Energy Eigenvalues for Graphene

$$\bar{a}_2 = \hat{x}\frac{3}{2}a_0 - \hat{y}\frac{\sqrt{3}}{2}a_0$$

$$\underset{\sim}{h} = \begin{pmatrix} \epsilon_0 & -t - te^{i\bar{k}\bar{a}_1} - te^{i\bar{k}\bar{a}_2} \\ -t - te^{-i\bar{k}\bar{a}_1} - te^{-i\bar{k}\cdot\bar{a}_2} & \epsilon_0 \end{pmatrix}$$

$$E = \epsilon_0 \pm t\sqrt{1 + 4\cos\left(\frac{\sqrt{3}}{2}a_0k_y\right)\cos\left(\frac{3}{2}a_0k_x\right) + 4\cos^2\left(\frac{\sqrt{3}}{2}a_0k_y\right)}$$

Choose $\epsilon_0 = 0$ show $E = 0$ at K, K'

$H \simeq A\bar{\sigma}\cdot\bar{k}$ massless Dirac

And we concluded with the band structure of graphene which is also shown in this viewgraph here. Here for example, this epsilon naught has been taken to be 0 which as I said is setting your energy scale. So, your Hamiltonian will become this 0 f K f star K and a 0, where f K is basically this kind of thing or we have done it already here.

So, either way you will finally get a spectrum which is this; which is the same as the one that is written here, the one that we wrote here this is the spectrum. So, one can then plot the function If this spectrum and as a as we showed the spectrum gives this kind of two states one coming from the bonding contribution, another coming from the anti bonding contribution.

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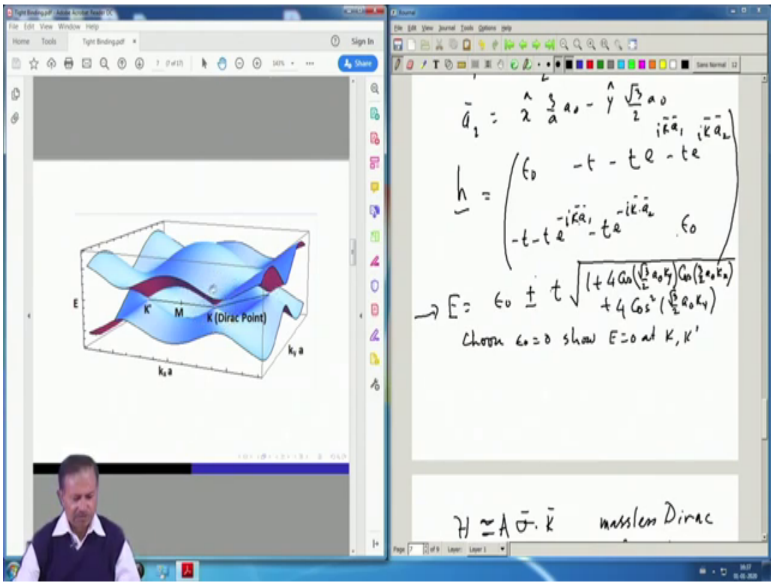

$\bar{a}_1 = \hat{x}\,\frac{3}{a}a_0 - \hat{y}\,\frac{\sqrt{3}}{2}a_0$

$$\underline{h} = \begin{pmatrix} \epsilon_0 & -t - te^{i\bar{k}\bar{a}_1} - te^{i\bar{k}\bar{a}_2} \\ -t - te^{-i\bar{k}\bar{a}_1} - te^{-i\bar{k}\cdot\bar{a}_2} & \epsilon_0 \end{pmatrix}$$

$$\rightarrow E = \epsilon_0 \pm t\sqrt{1 + 4\cos\left(\frac{\sqrt{3}}{2}a_0 k_y\right)\cos\left(\frac{3}{2}a_0 k_x\right) + 4\cos^2\left(\frac{\sqrt{3}}{2}a_0 k_y\right)}$$

Choose $\epsilon_0 = 0$ show $E = 0$ at K, K'

$\mathcal{H} \simeq A\,\bar{\sigma}\cdot\bar{k}$ massless Dirac

Now, there are other interesting systems that people talk about these days. Graphene of course, is famous for its to dirac points as we mentioned that you have a massless dirac spectrum at this these points linear in K in K and K prime. Whereas, the other interesting objects that have been discovered in the last couple of decades.

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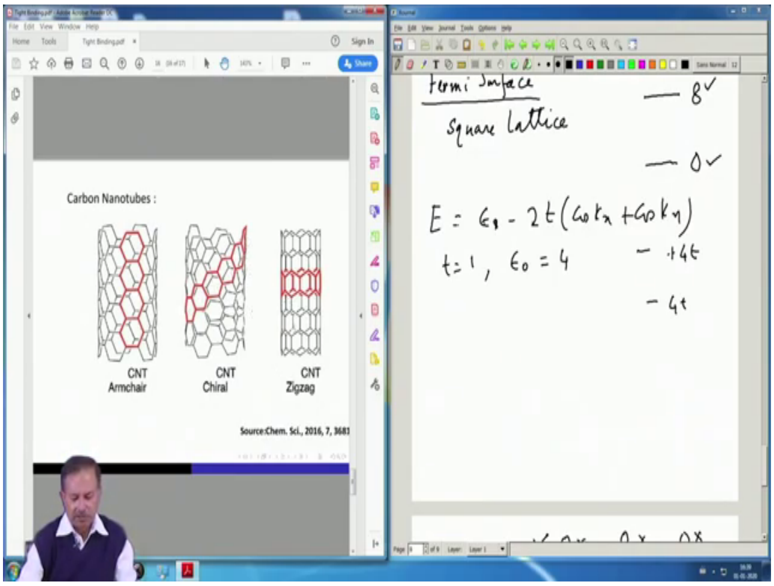
Carbon Nanotubes :

Source:Chem. Sci., 2016, 7, 3681

Fermi Surface

Square lattice

— 8 ✓

— 0 ✓

$E = \epsilon_0 - 2t(\cos k_x + \cos k_y)$

$t = 1, \ \epsilon_0 = 4$

— $+4t$

— $4t$

And these are really in our last 30 40 years these have become some of the major issues in research and major these are for example in a nano systems and nano sciences. These kind of small structures ultra small structures nanoscale structures are studied repeatedly and they are extremely important in terms of the applications a point of view.

Now there are two very common carbon nanotubes, carbon nanotube is nothing but a graphene folded into a tube. So, graphene sheet folded into a tube. So, although this came earlier than graphene, single sheet graphene singular graphene was only in the last couple of decades people have been able to use.

But this nanotube is in existence for a little more time this came earlier and there are two kinds of arrangements, as you can see these tube can be this the graphene sheet can be folded in two different ways three different ways actually. But these two are the major ones the armchair and the zigzag.

So, the name comes from this the red you can see the red part here and how these red part is arranged and in the chiral this is arranged in this fashion. So, and people have actually calculated their band structure. It is a straight forward to do it if you know how to do graphene you can also do this one.

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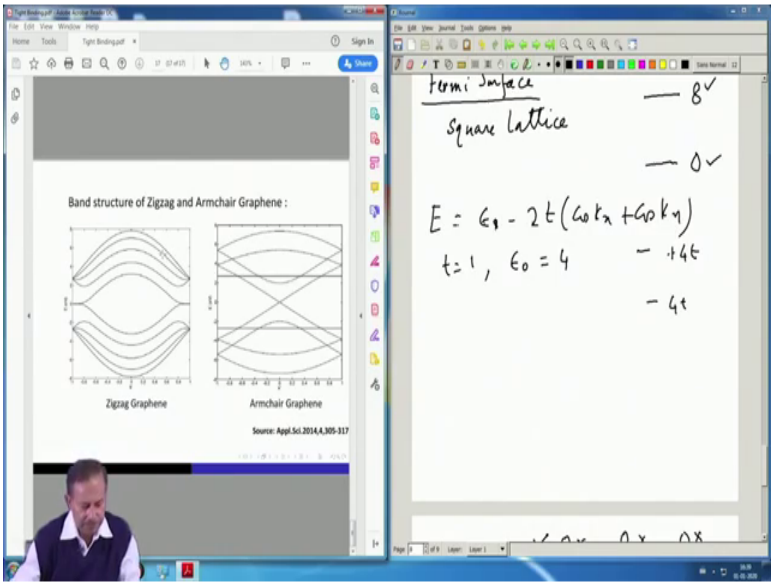

Band structure of Zigzag and Armchair Graphene :

Zigzag Graphene

Armchair Graphene

Source: Appl.Sci.2014,4,305-317

Fermi Surface

Square lattice

— 8✓

— 0✓

$E = \epsilon_0 - 2t(\cos k_x + \cos k_y)$

$t = 1, \ \epsilon_0 = 4$

— +4t

— 4t

And the band structure of these two are interesting, the look at the armchair graphene this has this point. Whereas, in the zigzag graphene you have the gap gapless regions here and here the band structure is completely different. So, that is interesting because it is a same structure just fold it two different ways and the band structure becomes completely different.

So, I will not belabour much on this, but this is just an illustration as to how different things can be by just changing the geometry a little bit. Let me also again go back to this point that I raised that there are instabilities of the Fermi surface.

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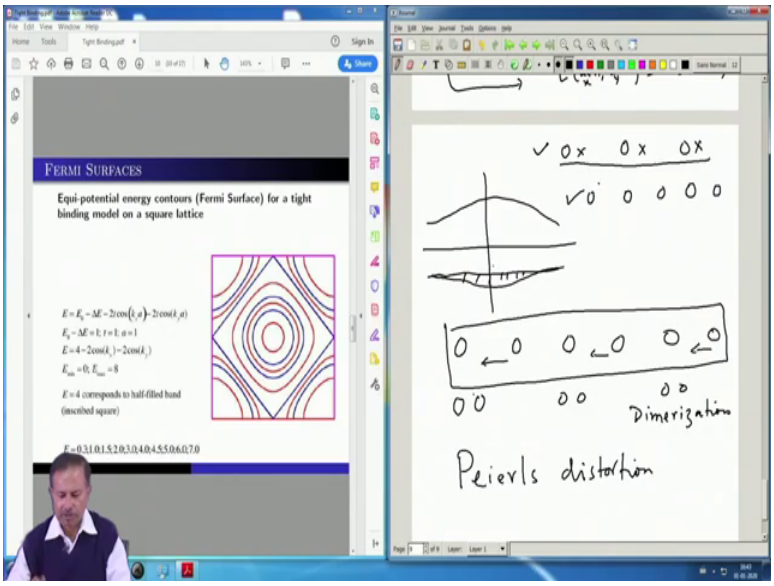

FERMI SURFACES

Equi-potential energy contours (Fermi Surface) for a tight binding model on a square lattice

$E = E_0 - \Delta E - 2t\cos(k_x a) - 2t\cos(k_y a)$

$E_0 - \Delta E = 1;\ t = 1;\ a = 1$

$E = 4 - 2\cos(k_x) - 2\cos(k_y)$

$E_{min} = 0;\ E_{max} = 8$

$E = 4$ corresponds to half-filled band (inscribed square)

$E = 0.3; 1.0; 1.5; 2.0; 3.0; 4.0; 4.5; 5.0; 6.0; 7.0$

So, Fermi surfaces of this kind for example. For example, this blue one this square Fermi surface this kind of Fermi surfaces are unstable towards distortions or other instabilities some longer range orders, because these kind of Fermi surfaces can be brought onto each other by just to look at this Fermi these Fermi surfaces this one the square one.

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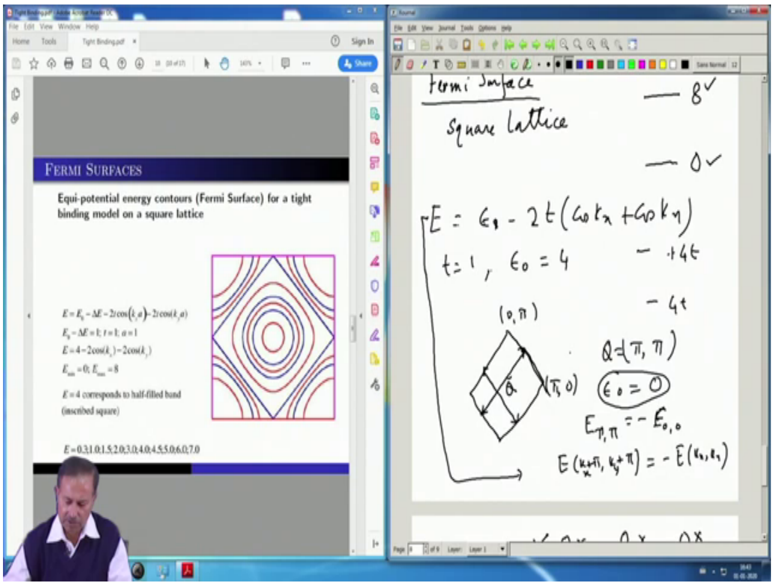

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Fermi Surface

Square lattice

$E = \epsilon_0 - 2t(\cos k_x + \cos k_y)$

$t = 1,\ \epsilon_0 = 4$

$— 8 ✓$

$— 0 ✓$

$— +4t$

$— 4t$

$(0, \pi)$

$(\pi, 0)$

Q

$Q = (\pi, \pi)$

$\boxed{\epsilon_0 = 0}$

$E_{\pi,\pi} = -E_{0,0}$

$E(k_x+\pi, k_y+\pi) = -E(k_x, k_y)$

So, this is pi 0 0 pi these points, now you can see that there is a Q vector and another one here. If you translate this one of these flat regions of the Fermi surface which is a line here by the Q vector then your and this Q is basically pi this Q here is pi pi.

And you can check for yourself that if epsilon naught equal to 0 then E at pi pi. So, what is so E at pi pi is minus E at 0 0. So, that means E of K plus pi K plus K x plus pi ky plus pi in this band; in this band structure at epsilon with epsilon naught equal to 0 epsilon naught equal to 0 this thing happens is equal to minus E f kx ky.

And that means these two energies just negative of each other and they are at the so these are at the Fermi surface. So, the both the energies are 0 so both are 0 here. So, this is for example, on this line so this is not 0 on this line, on this line your energy is 0. So, you can take an electron from here to here without changing the energy. But giving a momentum which is large which is like a reciprocal lattice vector. So, that is a it is a huge change in momentum, but no change in energy and that kind of situations lead to instabilities.

And one of these instabilities instability that I discussed is this one which we I called Peierls instability. Where what I showed is that if you have a regular lattice of this kind, that for example in one dimension in low dimensions that has a tendency towards forming a distorted lattice of this kind. This kind of distortions takes place and it leads to a dimerization and that is so what we are saying is in terms of band structure.

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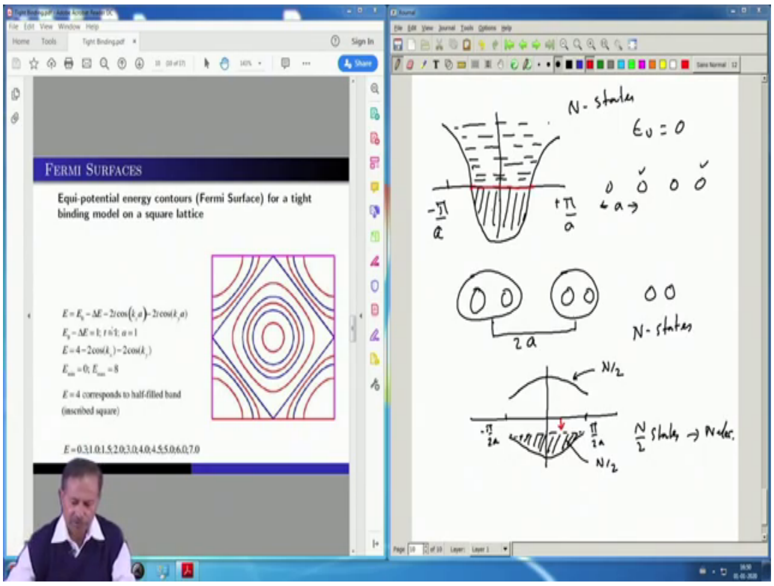

FERMI SURFACES

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We started with this kind of a band structure in one dimension for example, and we are half filled. So, our Fermi level is here. So, again epsilon naught is said to be 0 epsilon naught is 0. So, these are all field states at half filling and then this is for this kind of a geometry. So, this is pi by a minus pi by a and this is the distance lattice constant is a.

So, what this distortion does is that for example it will bring two of them closer alternately. So, you can move this one for example alternative alternate site alternate lattice site alternate atom to the left or to the right it does not matter, it is an infinite lattice so you can do it either way they are equivalent.

Now the this means that your unit cell is now the lattice constant is now twice and this kind of thing means that your Brillouin zone has now become half. So, let us go back to the picture that we drew earlier, in this kind of situation two atom per unit cell you will have this band is going to change to a band like the two bands which are like this.

And remember how many states we had? Here we had N states, how many states we will have here we will still have N states because the number of orbital's have not changed is N; N is still the number of orbital’s. What was happened is that the lattice constraint has doubled. So, your Brillouin zone boundaries are now at pi by 2 a and pi minus pi by 2 a.

And you have N by 2 states here and N by 2 states here still N states, because the Brillouin zone has halved you have a half number of states K values available for you. So, each of these bands will carry half the numbers. So, how many electrons can N by 2 states accommodate right it can accommodate N electrons.

So, I still have N electrons number of electrons has not changed. So, I will accommodate N electrons here. Now let us compare these two graphs , this one for example the top one, here is a metal because you have a states available up to this all these states are empty and there is almost no gap at the Fermi level. So, this is the Fermi level.

Here it has become an insulator. So, this is a situation which is energetically favourable for it and it has gained a large amount of energy by pushing down these this occupied part of the band down from here to here. So, there is a so each of the electrons are gaining a lot each of these N electrons have now gained a lot of energy electronic energy.

And that means this is the most stable state than the previous one. Of course, if you have a distortion that distortion is always that means that there is a lattice is strained. So, the lattice of course will contribute positively to the energy lattice energy will go up. So, that is kind of half K x square energy that will have to be added and but you can actually do the calculations and it is almost always that this electronic energy wins in a low dimension.

And therefore what Peierl showed was that he added the electron lattice coupling to it to the theory also and he found out that this kind of an instability is a rampant in a one and a two dimensions. And so this means that a freely floating one dimensional lattice without supported by anything is very hard to stabilize, it will tend to dimerize or lead to some distortion.

So, there the energy is gained and often it becomes an insulator. Similar thing happens in two dimensions one example I have just shown on the left that is this kind of a situation. Where if you have this flat regions of the band then you have, then of course you have a propensity for the system to distort the lattice and obliterate the Fermi surface. Basically make a gap produce a gap at the Fermi level.

So, this is a one route by which we can have an insulator. Of course, in this purely band picture you can have an insulator simply by having two bands for example.

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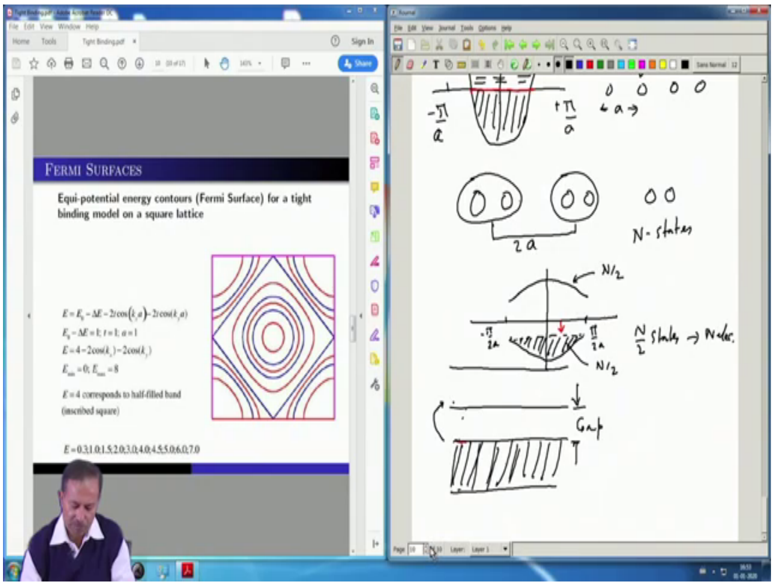

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$E = 0.3, 1.0, 1.5, 2.0, 3.0, 4.0, 4.5, 5.0, 6.0, 7.0$

If you have just two bands say for example, one coming from your s orbital's and another coming from p orbital's and so on. You can have two sets of bands one is occupied and then there is a gap and so any so these are all occupied states. To excite an electron you have to take the electron from here that is the minimum excitation energy then you have to put it here. And that means, the finite energy required for the electron to be shifted up and that is a situation which is basically you can see that it is nearly incompressible.

And to put even to change the number of electrons by one you have to have a finite energy. Suppose you want to put in an electron from outside and make it N plus 1, then you can only go here at the top band and the bottom of the top band which is empty and that means, there is a gap to that. So, finite energy is required to either excite or add an electron to the system.

So, this is how in the band picture the picture that I have just shown you, this is how metal to insulator a metals and insulators or semiconductors are distinguished. It is simply a single particle levels where you have two levers two bands formed out of two different sets of orbital’s. They can mix also weekly sometimes they weekly mix because a orbital’s are not orthogonal at different sites.

So, but then finally you will have the number of states remains the same. So, you started with two orbital’s per site you will get two sets of bands. And if there is a gap in between them and if you are filling density is such that you fill the lower band and keep the upper band empty then you are having an insulator. And that is the picture of formation of an insulator in the you know in any of the band structure the theories that one does. Of course, the band structure that we did is the simplest.

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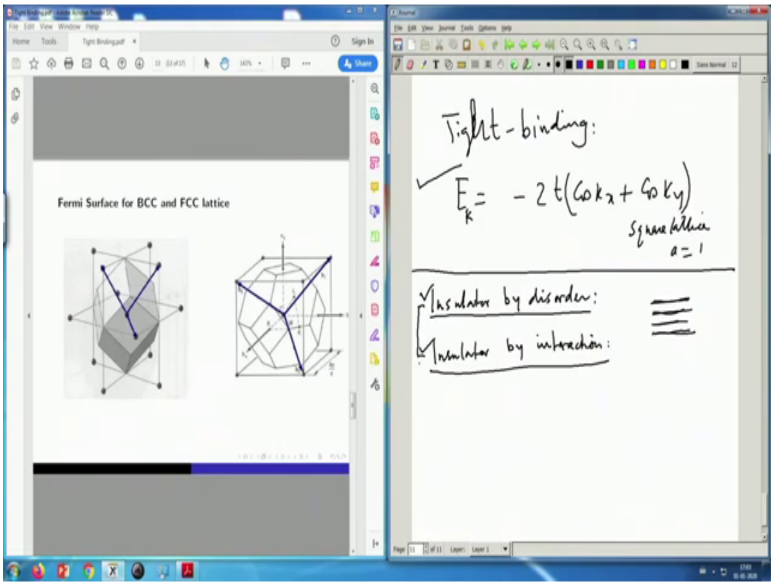

Fermi Surface for BCC and FCC lattice

Tight-binding:

$E_k = -2t(\cos k_x + \cos k_y)$

square lattice

$a = 1$

Insulator by disorder:

Insulator by interaction:

So, this is the tight bind tight binding, in tight binding approximation you saw that for the square lattice. For example, E is a minus 2 t cosine K x plus cosine K y E of K E of K. Now, this is a again set episode not equal 0 this is the simplest.

For example, for a for square lattice for a square lattice this is square lattice with a equal to 1, this is the band structure and then a and t is the hopping matrix element. So, this is the simplest that one can do and from the simpler simple picture one can get a lot of insight about the nature of the material. That one is considering whether the material is an insulator or a semiconductor and so on and so forth.

So, this kind of very simple pictures it can also tell you about the Fermi surface. For example, these are Fermi surfaces for BCC and FCC lattice. So, if you know the density if you know how many electrons you have to accommodate and then you calculate a band structure and just fill up the states.

So, that is the beauty of doing this a single particle physics, because you will be solving the Schrodinger equation for only one electron in these entire set of orbital’s and in this the Hamiltonian that we wrote down. And then obviously we neglected the electron interaction you also took the Born-Oppenheimer approximation where the nuclei is considered fixed under that approximation particularly without any interaction between the electrons these this is the way one has to go about solving the band structure. There are more complicated ways of doing the same thing. There is a method already well develop band structure methods this is that is a very sophisticated technique.

But the ultimately at the end of the day what they do is still calculate the single particle energy levels and put particles add those energy levels and that is still the procedure. And if you there are so called density functional theories and so on which has a very celebrated theories earned a Nobel Prize also. And there also people tried to take care of certain kinds of interaction between systems.

But at the end of the day it is again a single particle picture in which you will have single particle levels, which you have to fill up starting from the bottom. Now of course, this is as an aside this is not the only method by which you can get an insulator from a metal. There are two more well known categories which are one is by disorder. So, insulator by disorder and the other one is an insulator by interaction.

The first one was worked out by PW Anderson and the second one had contributions from many people, but the this it is goes by the name of Mott transition. Where in the first one what happens is that you if you put disorder in the system, of course the calculation that we did the Bloch theorem that we used, those are usable only if you have a perfectly crystalline system.

If you deviate from perfect crystallinity suppose you put some defects some substitutions or some defects that naturally creeping inside a system. Then you have no choice that there would be some effects of that and that if it can be dramatic in dimensions less than or equal to 2 and that was shown by Anderson and the collaborators.

And what they showed is that any final disorder in dimensions two and below can have catastrophic effect. And in three dimension they can also have effect depending on how strong the disorder is. There are many kinds of disorders not just defects you can have boundaries you can have domains and so on and so forth or external impurities or damage by the radiation and so and so forth.

So, all kinds of disorder, but all of them will have the salutary effect that in dimensions two and below, they can change the nature of all the states dramatically. These are still single particle states these states dramatically change their character and that character that is that these states are no longer extended states like in the block theorem that we got, plane wave extended states and these become then localized.

So, the nature of the states change and that is called the Anderson mechanism for Anderson's mechanism for disorder induced metal to insulator transition. So, as you increase the disorder slowly and slowly this the states start to become localized and in three dimension at a critical disorder you will finally localize all the states.

And then no state will span the entire remember the plane wave states that we are studying with they are equally probable to find almost everywhere in the in this in the system, because they are plane waves. So, these states are they are everywhere. So, the that nature has changed and the state that one lines up with a disorder are localized they are exponentially decaying and so that is one mechanism by which you can have a insulator from a metal starting from a metal.

There is another one which is more much more complicated which is as I said is driven by interaction between electrons and this is of course, not describing in the same way that we did this band structure calculation so far. Because now we because you have interactions you cannot write a wave function of a multi particle system as a product wave function starting from single particles.

So, this filling of bands this filling of levels and comes the idea that there are single particle states breaks down in this when interaction is present and this leads to a very dramatic leads to very dramatic new physics in the in many systems. Particularly systems where the electrons are in 3d or 4d or three or 4 f or 5 f levels the valence electrons, they are the electrons are tightly bound to the nuclear to the parent atoms.

And so the effect of interaction is dramatic, because their bandwidth is low and it can lead as the interaction increases one can completely use this single particle picture. So, that is a completely different scenario and we will not discuss it further. But I just want you to remember that there are other mechanisms by which insulators can form.

Which is one is this insulator by disorder and other is by interaction. Then the then of course, the nowadays you must have heard of things like topological insulators and so on. these are fairly advanced topics they are interesting and these are some of these topological insulators. For example, are insulators in the bulk and they have metallic states at the surface. So, and these are effects these effects these effect is dramatic also here and there lots of very interesting physics that are coming out.

But we will probably discuss those things at a later stage when we discuss some advanced topics towards the end. But at the moment let us just know let us just remember that there are these new states that are new physics that is coming out. And this old this way of doing a physics with the electronic physics with the only the conventional band structure works very well in most systems in many systems.

But it may fail in certain cases and that is where some very interesting new physics has come up in the recent years and for last 50 years or. So, one knows these other routes of metal insulated or transition and so on. Those will not discuss in this course, but topological insulators we might discuss as an advanced topic towards the end.