Introduction to Reciprocal Space
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Lecture -08
E Vs k, Brillouin Zones and the Origin of Bands

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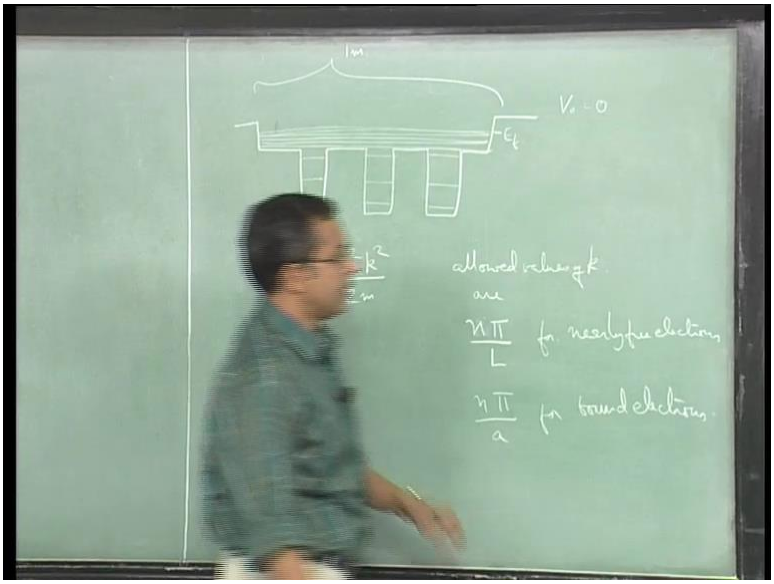

In this class, we are going to pull together lot of information that we have seen in the last few classes. And understand how we can predict material properties based on our analysis that we have developed and these skills that we have developed to understand how the material behaves, how the constituents of the material behave.

So, we finished off with a diagram which wherein I showed you the fact that you know on the same diagram we can put together the reciprocal lattice information as well as E versus k information. So, we will start our analysis just one step behind from there and then proceed forward. We will look at how nearly free electrons interact with the lattice and we will do this in considerable detail in one dimensions.

In, one dimension because that is easier to understand and easier to represent on a on the plane of a board. So, we will do that in significant detail I will show you also on the board how the same information can now be represented in two dimensions. And finally, we will look on at a few

slides where we are looking at the same information, the same kind of interaction for a material in three dimensions.

Now before we start drawing the diagrams and looking at the interaction I must tell you that you know when we actually finally built up this model using the Fermi Dirac statistics. Importantly we identified something called the Fermi energy which is the energy of the highest energy level electrons right. So, we also noted that everything is filled up to that energy level and that is the first set of the highest set of electrons present in the system.

In terms of energy and therefore any interaction that you see with the outside world so to speak, is based on what those electrons can do okay. So initially we will draw the diagrams without bringing in the Fermi energy then we will show you where the Fermi energy is and then let us look at what is represent okay. So, let us start from something that we are familiar with and we will proceed from there.

I said that our, we should understand clearly what we are drawing, so that is why I am to show you something and reiterate something that I have mentioned before and then you can follow the diagrams much more appropriately fine. So, this is the simplified model for our system that we are using and we have seen this a few times right. So, this is V equal to 0 wherein the electron is at infinity and therefore its potential is 0, V0 is 0, 0 volts if you want to call it that.

This is the potential well that corresponds to the extent of the solid. This represents electrons which are trapped within the solid but still are free to move through the entire extent of the solid. They are not really confined to any one atom or any one ionic core and then these potential wells represent the potential, narrow potential wells which are potential wells corresponding to each individual atom okay.

And therefore, the electrons that are trapped here now are localized, if that is the term that are used. They are localized to that particular atom right and in terms of energy levels these are some energy levels that they can have, so we have just these are all this is just a schematic, so I am just showing you something here. And then there are a large number of energy levels here which are very closely spaced okay.

This is a schematic, we have to show something on the plane of the board and that is the way it is shown. To give you a again the widths here are 10 power -10 meters, the entire dimension here is of the order of a meter. I mean this is just a, to give you a scale of what we are looking at okay. And regardless of, so in fact if you looking at 1 meter, since this is only a schematic.

As you can imagine, in 1 meter you can have 10 power 10 such atomic cores so to speak of or maybe half of that, half as many if you are assuming the gaps are roughly similar. So, I have just drawn 3 here, so obviously this is just a schematic, so this is not really, it is not that there are only 3 atoms in this 1 meter length okay. So, there is a huge number of atoms, if this is for schematic purposes.

In terms of localization the basic concepts of what happens when you localize is still the same regardless of whether you are talking here of the electrons at these energy levels or at these energy levels. And basically, localization means the energies are now quantized which means only specific values of energy are permitted for each of the electrons.

And those energy values can now be represented in terms of the allowed k values because energy and k are related like this. Therefore if, only specific values of energy are allowed, only specific values of k are allowed, in fact it when we do the calculations it works out the other way. We learn that only specific values of k are allowed for the system once you localize it.

Therefore, only corrupts those corresponding values of energy are allowed for this, for those electrons. Now the allowed values of k are 2pi, I am sorry are npi by L for nearly free electrons and npi by a, for bound electrons. And the difference is, the as you can see the form is exactly the same npi by some length dimension here.

And the it is only the question of whether this length is one meter, if it is for a nearly free electron or it is a which is sort of the atomic dimension which is here okay. So that is the difference between the two of them, so for both of them we can draw curves representing the allowed values of energy. So, I will, so that we now have in sense three cases, two of them are listed here.

The third one is for a nearly, for a completely free electron which has escaped the solid okay. So, for that all values of k are allowed, there is no restriction any value of k. Therefore, all values of energy allowed and this here the highest energy value here is Ef, the Fermi energy that we spoke about.

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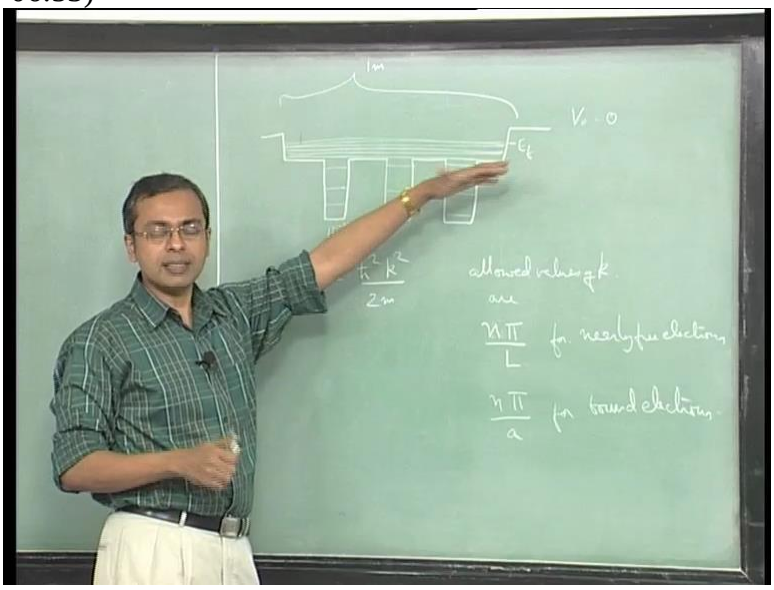

So, we will draw all the three of them and then we will make a quick comparison E versus k here, this is E, this is allowed values of k. So, for a free electron, so this is free electron, this is nearly a free electron okay, so this is k again, this is E. Now only discrete values are allowed and those values of k are npi by L, so this is pi by L, this is 2pi by L, this is minus pi by L, -2pi by L and so on okay.

And this is for a bound electron, so I just put it here, E k bound electron, so this is npi by a allowed values of k, so this is pi by a, this is 2pi by a, this is -pi by a and this is -2pi by a, correspondingly you will have allowed values of k, I mean energy values we can have further values somewhere there okay. Since the relationship is still h bar square k square by 2m the energy versus k. The, if you connect this dot you are going to get a parabola.

So that therefore the shape is the same as that for a free electron except that several points here are now no longer valid. Only specific points along this curve are valid and that is what we see both for a nearly free electron and for a bound electron. So, this is how these three figures relate

to each other. Now the important thing to notice the scale of this is very different from the scale of this okay.

So that is the important thing to note, so for example this pi by a, because this is a of the order of 10 power -10 meters, this is now in the denominator, so pi by a is actually a very large value relative to pi by L, which is, where L is of the order of a meter. In fact, there are, if you plot this figure on this scale then between the origin here which is 0 here, between the origin here and pi by a.

There will be 10 power 10 points corresponding to allowed values of this nearly free electron okay. So that you just need to keep that in mind for to understand the scale of these two figures. I am not going to, I am right now this is a separate figure this is a separate figure, I am only drawing a comparison between the two, so that you are aware of the scale of it okay. So, you have to keep in mind the scale of it the form of the equation is the same.

So, you still get pi by L, pi by a so that is still the same except that a, is 10 power -10 meter, so this is a, and it is in the denominator, so this is a very large number, so it is pi times 10 power 10, this is simply pi. So therefore, if you take the same this information and you plot it to this scale then you will find that there are 10 power 10 points between 0 and pi by a, if you look at this figure or another or to put it in another way.

If you look at pi by a, here on this scale, you have to go, you have to add 10 power 10 points here, I have only put 2 points here okay. So, I have only put 2 or 3, 4 points drawn out here, you have to go up to 10 power 10 points on that side before you get the first pi by a here, that is the difference in scale between this figure and this figure, so this is something we keep in mind now.

So, this is all with respect to the electron, what is our goal? Our goal is we will look, go back to our previous figure and we will see what we are trying to do? We would like to understand what is the interaction between the allowed values of k corresponding to these nearly free electrons, so there are k values of these nearly free electrons, what is the interaction between the allowed values of the, k values of these free electrons with the periodicity of the lattice okay.

So, lattice has some periodicity okay, so this is a different piece of information, I right now in our immediate in our, in the discussion we are going to have now, we are not really concerned about these bound electrons okay. So, we are not really concerned about bound electrons, we only talk about the k values of the free electrons or nearly free electrons.

We only talk of the k values of the nearly free electrons but we will look at the interaction of those k values with the periodicity of this lattice which is still of the order of a okay. So, I have, the previous comparison I do drew was simply to show you that the scale of a versus L, but and so therefore we are still going to use this a, which is the periodicity of this lattice.

Except that we are not talking in terms of the boundary but this periodicity between this point and this point, this point and this point, it is still of the same sort of order of magnitude as these width's okay. So that is where the scale comes from, roughly we get the scale okay. So that is how we look at it.

So, we are going to look at the periodicity which is now coming from, which we are, we discussed in the last few classes is being represented in reciprocal space using reciprocal lattice information, reciprocal lattice designation okay, denotation. So, the reciprocal lattice will capture the information of the periodicity of the lattice in that in the reciprocal dimensions. The k vector will catch capture the information of the allowed wave vector in reciprocal dimensions and we will look at the interaction between the two of them.

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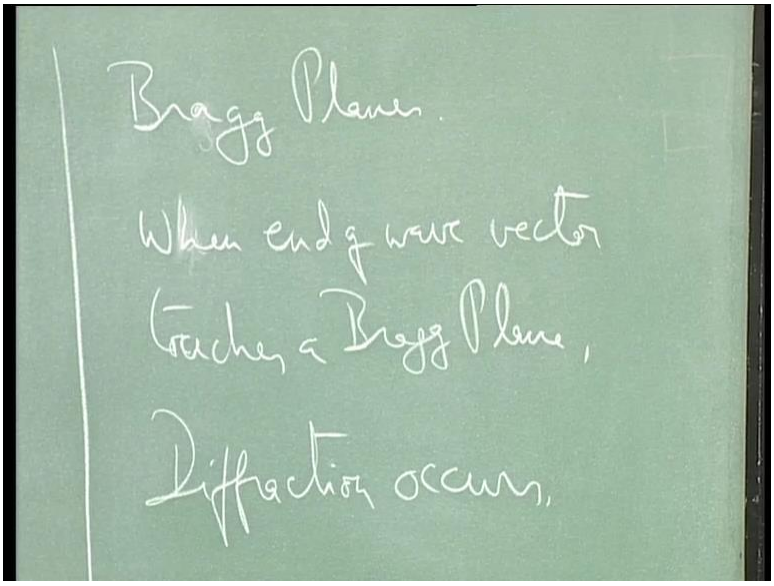

In this context, we also saw, so I put that down reciprocal lattice information of periodicity of lattice in reciprocal units and k vector information of allowed k and energy values. And therefore, energy values in reciprocal units okay. So, this is k vector captures information of allowed k and therefore allowed energy values in reciprocal units.

And this is reciprocal lattice which captures the information of the periodicity of the lattice in reciprocal units of the structure right. Only differences in the manner in which we discussed it, this is a lambda is being represented as 2pi by lambda here and here a, was being represented as 1 by a. So, the difference is that there is a scaling factor of 2pi okay.

So, I will just put an arrow here so lambda is represented as 2pi by lambda, a is represented as 1 by a, we talk of this interaction in the context that we say that we are representing everything in k space, the diagrams we draw is drawn in k space, what is k space, k space is one where the all the information is being represented in this form okay.

So therefore, any dimension in any length that we see in real space, we are plotting it as 2pi by that length in the reciprocal space okay. So that is the sort of the convention we are going to follow. Therefore, if you represent the reciprocal lattice information in k space again we will scale it by a factor of 2pi and that simply a multiplicative factor.

It simply means that you are only changing the, you are multiplying, you are not changing the symmetry of the structure that you see. You are simply changing the scale of the structure either

in this case your magnifying it because you are multiplying it by 2pi okay. And it is, it does not change anything fundamentally because we are representing two pieces of information on the same scale which is all we are really interested in.

We are able to look at the interaction only if all the information is represented in the same scale therefore it is necessary to do that. So, we represent reciprocal lattice also in k space and allowed wave vectors also in k space and we will look at the interaction okay, so that is what we are going to do. What is the additional thing we have done? We have seen that in reciprocal space we have identified what are known as Bragg planes.

And we have said that when a wave vector, when end of a wave vector touches a Bragg plane, then diffraction occurs okay. So, when the end of a wave vector touches a Bragg plane diffraction occurs. So, these in fact are captures the interaction that we are going to look at, basically we are saying this Bragg plane is coming from the reciprocal lattice okay.

So that belongs to, that represents now the periodicity of the structure that we are discussing. The wave vector that we are talking of belongs to the waves of any radiation or electrons that are present in the system that are interacting with the system. In this case these waves, these are the wave vectors of those nearly free electrons present within the system.

The interaction therefore of these wave vectors with the periodicity of the lattice is captured by the fact that a specific values of wave vector, when the wave vector touches a Bragg plane diffraction occurs. And corresponding to the diffraction process what happens is certain amount of, certain values of energy now become forbidden okay.

In fact, what happens is when diffraction occurs that E versus k relationship gets distorted very, very near the diffraction condition. As a result, certain energy values get are prevented from occurring. What we will do in this class is we will look at this pictorially, in the next class we will actually put down values, we will look at how we can solve it sort of analytical fashion, we will see what equations we can put together and see this in a mathematical sense.

So today right now we will look at it in a pictorial sense okay, so that is how all this comes. Again, wave vector is in the 2pi by L scale or npi by L is the scale for this. This is Bragg planes

which are 1 by a, and now 2pi by a, okay. So again, you see that it is something with a in the denominator, on that scale we are going to plot something with L in the denominator. So therefore, you will see this. So, on this scale it look like a continuous set of point, so that is what we are going to look at.

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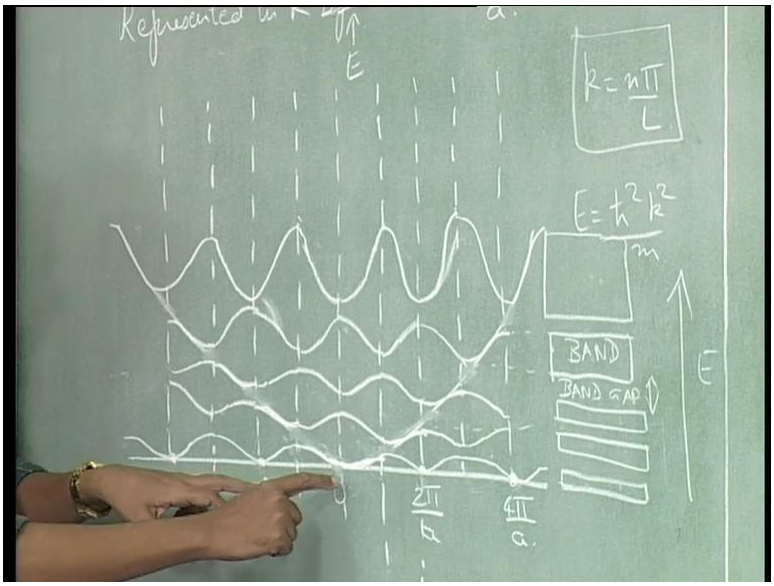

So now we will look at a one-dimensional lattice okay. A one-dimensional lattice with spacing a, inter atomic spacing a. Now to represent this in k space, represented in k space, a will now get represented as 2pi by a. If it was simply reciprocal space in the manner we originally discussed it a, would have been represented as 1 by a.

We are representing specifically in a particular scaled version of reciprocal space called the k space but the scaling factor is 2pi so a, is going to be represented as 2pi by a. Therefore, reciprocal lattice vectors, once you start, so once you identify an origin for this k space, reciprocal lattice vectors at, occur at intervals of 2pi by a okay. So therefore, we will plot that up here okay.

So, we will just say that this is your scale, axis this is the origin okay so reciprocal lattice vectors occur at 2pi by a, 4pi by a, okay. So, for the moment we just take 2, 2 points so that that keeps the image rather clear, again -2pi by a, and minus 4pi by a. So, this is the information, this is the representation of the periodicity of the lattice in k space. Lattice of periodicity a, has now been represented in k space with these four points.

I have just taken four of those points and represented them here okay. So that is all we have done we including one and they include the origin so five points if you wish. Now we have we have a few things to do we would now like to identify the Bragg planes okay. So, then we know where it is that we can look for diffraction. So, let us see independent, so with respect to this periodicity let us identify the Bragg planes.

So, what is the Bragg plane? Bragg plane is the plane that bisect the perpendicular bisector to a valid reciprocal lattice vector that is the Bragg plane. So, we look at the origin, the valid reciprocal lattice, first valid reciprocal lattice vector is at 2pi by a, so half of that is where the Bragg plane will occur. So therefore, the Bragg plane occurs at pi by a, okay. So, this is where the Bragg plane occurs, first Bragg plane.

So, we will just draw a dotted line which represents this Bragg plane okay. So that is a Bragg plane in other words on this plot or in k space, if we plotted all the allowed wave vectors when the wave vectors arrive at, a wave vector at this value would now imply that the wave vector is touching the Bragg plane implies the diffraction is occurring. And that causes distraction of, distortion of that E versus k relationship.

And you start seeing some energy values which are not allowed in the system. So now, it so this is the information, so we have the first Bragg plane here, the second Bragg plane this is at 4pi by a, at half its, so that is the next valid reciprocal lattice vector, so at half the distance you should have the second Bragg plane which will actually come at 2pi by a, so that is where you have the next Bragg plane.

Similarly the next one will be at 6pi way, so therefore a 3pi by a we will have another Bragg plane, essentially at every npi by a we are going to have a Bragg plane because at every 2npi by a, we are having a lattice point. So, this is what we have, same thing we can do here, so we just mark this up for the origin okay. So now I have plotted all the Bragg planes in the system, I have plotted the periodicity of the lattice.

Because of the periodicity of the lattice, I have plotted all the Bragg planes. Now, so this is k space, on this very same plot, I can take the nearly free electrons and plot their wave vectors

okay. So nearly free electrons are electrons where the allowed values of k are npi by L. So, we notice that this is npi by L here the same discussion that I had earlier which means you have 10 power 10 points of such 10 power 10, I have points of this npi by L.

Within this distance 0 to 2pi by a, so therefore even though I will, which basically means that you know on this scale when I show it to you, it will look like a continuous curve, the reason I am emphasizing this is I am going to draw a line that looks like, I am going to draw something that looks like a continuous curve. But you must keep in mind that it is not a continuous curve it is a set of discrete points which are all spaced by this npi by L.

Except that their source closely spaced that we are unable to show them as discrete points on this scale that is all you need to keep in mind okay. That these are discrete points the curve that I am going to draw consists of discrete points but they are so closely spaced on this scale that it looks like a continuous curve okay. So that is what we will, these are the allowed values of npi by L.

So, the discrete set of points will now have this, the original E verses k relationship is E equals h bar square k square by 2m. So that same parabolic curve like thing we will draw here okay. So, this is an approximate parabola, may not be the best parabola but you can still see the basic idea here. So that is the parabola we have of allowed values of E versus k, which are now drawn to this scale okay.

So, this is the parabola if you draw it properly you will get a nice parabola that corresponds to the E versus k relationship of the nearly free electrons. So, it consists of a series of discrete points several, several huge number of points all spaced by npi by L, which on the scale looks like a continuous curve okay so that is what we have. Now based on what we have understood all the things that we have learned so far, what we what we learn is that?

Whenever this E versus k relationship touches, these are all valid reciprocal, I am sorry these are all valid wave vectors. Whenever a wave vector touches a Bragg plane diffraction will occur, conditions for diffraction are fully satisfied. So therefore, diffraction occurs here, here, here and here. So, what actually happens is this E versus k relationship now gets broken up at those locations where the diffraction is occurring.

And essentially is described by saying that you know travelling waves become standing waves so to speak. So, what will happen is this relationship will now change and the diagram will begin to look like this okay. So, this is how the diagram now looks, it means that suddenly you have a few locations where the E versus k relationship is now no longer what it used to be before.

So, we can just remove some of these points here and you can see it little more clearly okay. So, these now are the allowed values of E versus k, so you see now what was originally a parabola at regions where it comes close to the Bragg plane that parabola is now being distorted and we actually end up seeing some discontinuities. You see the E versus k which should have just gone up this way because it has come close to a Bragg plane distortion becomes like this.

Similarly, it starts from some value up here goes this way gets distorted and finishes off here. Starts here finish off here, starts here and finishes off here, same thing occurs this way. And so in between where it was originally a continuous curve the interaction of the periodicity of the lattice with the k vectors representing the wave vectors allowed for the nearly free electrons.

We find that the nearly free electrons, so now if in other words if you go back to this figure here, the nearly free electrons the k vector of these nearly free electrons undergo diffraction due to the periodicity of this latter okay. So here we capture the fact that you know when diffraction occurs we are looking at the interaction of electromagnetic waves with the periodic structure of the material lattice.

And as we are somehow used to thinking that this the waves involved are coming somewhere from an external source that is because that is how we do the material characterization, we look at electron microscopy or x-ray diffraction. So those, in those conditions the waves are coming from outside the sample, however to the extent that you can look at electrons also as waves.

The electrons within the solid themselves represent waves and wave vectors and they to can therefore interact with the with the periodicity of the lattice using the same relationships that hold for the other material characterization techniques that we look at. And therefore, that is basically all that we have seen here, diffraction is occurring at those Bragg planes and as a result this energy verses and therefore as a result this E versus k relationship is now getting distorted.

So, this is basically what we see okay. So, as you can see now if you look at the vertical axis is the energy axis alright. So, in this energy axis we now see that because this E versus k relationship is getting disturbed, we find that we have a set of energy values which are continuous which are now allowed. Then there is a gap here which represents an energy that is not allowed okay. So that is like a forbidden energy gap here.

And then again you have a set of energy values that are allowed, the same thing can now be plotted like this. Now represents a set of energies that are allowed corresponding to this height has just drawn that on the same energy scale here. Then there is a gap, then there is another set of energy values that are allowed okay and then there is a third set of energy values that are allowed, this is fourth set corresponding to this okay.

So this is what we have, so what we see now is that from this picture we are able to see that there are specific sets of energy values that are allowed and specific sets of energy values that are not allowed, this is the picture that we are conventionally used to when we describe saying that we there are bands in a solid, energy bands in a solid and there are allowed bands and there are band gaps so this is a band gap okay, so that is the band gap and this is a band allowed band okay.

So, we now see based on all the understanding that we have pull together through this course, we are able to see how fundamentally the interaction of electrons with the periodicity of the lattice creates the situation where bands and band gaps appear in the system okay. This kind of representation by the way is called a flat band diagram.

Because a lot of the detail of the allowed actual allowed k vectors and such are not actually shown in this kind of a diagram but this is the kind of diagram that is typically shown to us in high school physics because it is much easier to follow. And in fact, for certain types of activities where we are looking at transitions and energy levels corresponding energy values associated and so on.

This figure, this kind of representation is adequate. There are certain other phenomena in the material where this representation is inadequate and we will see that in a class or too in a couple of classes we will see that, that this level of detail that this figure represents actually gives us a

much better understanding of what is allowed in the system and what is not allowed in the system, what is more likely to occur and what is less likely to occur?

And how two materials may differ from each other okay, so these are the allowed bands and these are the band gaps in between them. These are, this is a band gap, band gap, band gap and band gap and these are all allowed bands. So, this is how something that you have always learnt in high school now relates to something that is much more intricate, much more detailed about the system okay.

So, we see now all the things that we have put together and represented it here. I will also say that if you look at this diagram this kind of representation is called the extended zone scheme okay. Extended zone scheme where you take one origin and you draw the entire reciprocal lattice about that origin. And then on that basis you actually draw this entire diagram okay. So, this is called the extended zone scheme this is called the flat band diagram.

Now there are a couple of other ways in which you can represent exactly the same information so I will on this diagram itself let us see if we can pull that information together, so that you can see what we are meaning, representing. It is a basically the same information, now the information is already on the board, we are not really changing the information I am just showing you certain other aspects of the information.

Which may not immediately be apparent because of the way we have drawn the diagram, the information is that see this choice of origin is somewhat arbitrary, it is our choice we select by our convenience, so therefore we can select the next lattice point also at the origin, the next reciprocal lattice point also as the origin and so on right. So, there is no real difference between these lattice points in that sense.

Therefore, the same diagram can be shifted to the right by one reciprocal lattice vector, can be shifted to the right by two reciprocal lattice vectors and similarly to the left by one or two reciprocal lattice vectors. So, in fact it is correct to actually say that this exact same situation exists about every reciprocal lattice point. Because there is, our choice of origin is rather arbitrary; we have just chosen one for our convenience.

So, what we will do is we will draw the exact same diagram about this lattice point as well as this lattice point, this lattice point, as well as this lattice point okay. Then when you do that you will see what will happen. So, about this lattice point you see this curve here the same curve will occur here and the same thing will occur about this lattice point, you will see that also, same thing will occur here and will occur here fine.

Now the next what you see here as the next feature will also occur similarly across every lattice point. So, you will see that, so basically if you look at the second lattice point, you have drawn this curve here. The next structure will start here and go up here, the next one will start here and go up here and the next one will start here and go up here and then the next one starts here and goes up it.

So, this is the same diagram now drawn from this point and similarly you can take the next point here and it will come up here. Now I can draw the same diagram from here, the same way we have done which will look exactly like this okay. So that is what we will do and we can do similarly from all those points from this point. We can do the same thing we have got this so the next curve will look like this.

The next curve will look like this and the next curve will look like this fine. And we will do that also from this point here, so you will see how this figure begins to look okay. So basically, this curve now builds up across all positions that we have considered. So, what you will see is, you will see a series of curves that look like that coming from all different lattice locations okay.

So that is how you will get it, this will come all these diagrams that I am drawing will now come from the adjacent positions that we have seen. You just have to continue this diagram, use the same logic and you will start getting this kind of a diagram okay. So, we have that and you will see that this will come down here, this is coming from some lattice point from that side you are coming, you are bringing it that side.

That is how this will become; this is how it will come okay. So now you see that same information what we originally drew up, about one lattice point which was the origin, I have now drawn from every single lattice point that is across this structure and so they all begin to, they

also show you some pattern here okay. That is simply because the same pattern is originating from all of those locations.

And this pattern now represents this band okay, so this is like this bottom most thing which is going this way, this way, this is represented by this band as a flat band diagram. The same thing here represented by this band, what is here is represented by this band, what is here is represented by this band and similarly what is up here is represented by this band.

In between you see this gap; these are all not energy values that are not allowed that is the band gap. This is all not allowed another band gap, again these are all not allowed third band gap and this is one more band gap that we have it okay. So, this is another way of basically the same information has now been shown to you from the entire lattice. So, you can actually draw this across this entire lattice you will find such diagrams.

That is called a repeated zone scheme okay. So, this is called repeated zone scheme representing this information from across all lattice points. Finally, we will also notice that if you look at the, what we originally defined as the Brillouin zone okay. The Brillouin zone is when you are, when you the first Brillouin zone is the region in space which you can access from the origin without causing a single Bragg plane right.

So therefore, if you look at the Bragg planes here they are at, the first Bragg plane is at plus pi by a and the side at minus pi by a. So, the first Brillouin zone is actually between, so we will write the Brillouin zones down here okay.

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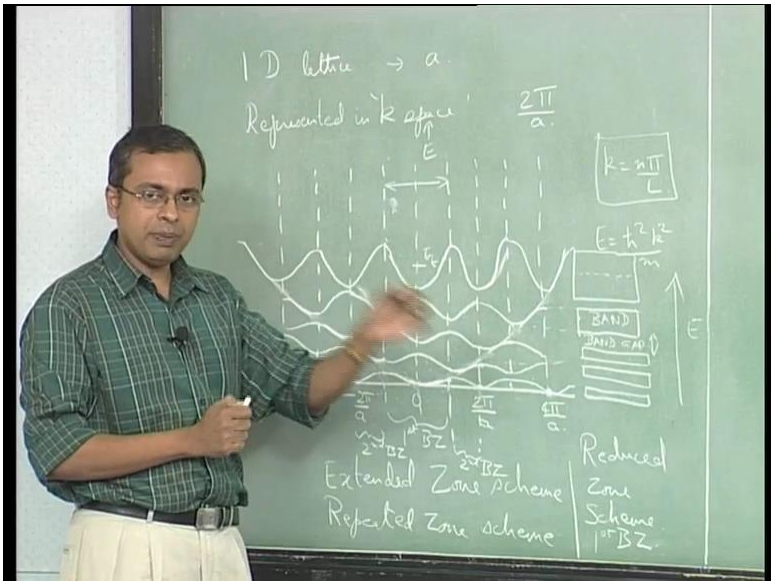

So -pi by a to + pi by a is what the first Brillouin zone is and we will, I will show you that. The second Brillouin zone is some -2pi by a to -pi by a as well s +pi by a to +2pi by a in both cases you would have crossed one Bragg plane but not more Bragg plane. So, if you come here the first Bragg plane is here, so this region then is the first Brillouin zone, I just call it first BZ, first Brillouin zone, this region here plus this region here together other second Brillouin zone right.

So, we have the first Brillouin zone and the second Brillouin zone, if you add the two second Brillouin zones the total dimension is the same as the first Brillouin zone okay. So that way all the Brillouin zones when you look at them they may get fragmented into pieces. When you collect all the pieces together the extent of it will be the same as the extent of the first Brillouin zone.

So anyway, if you see whatever information we have captured in this repeated zone scheme. All that information actually exists within the first Brillouin zone itself right, so all the information in fact because of symmetry you can actually look at just the first Brillouin zone and whatever conclusions you can draw from the first Brillouin zone will actually be represented, will be representative of the conclusions you can draw if you drew it across the entire lattice.

And that occur simply because the structure is periodic and therefore whatever is happening is happening periodically. So, if you gather all the information within one zone, you will still get the same piece of information and you can see that that way the diagrams have come, if you

could look at just the diagram between this region and this region which is the first Brillouin zone, you look at it, the same pattern is only getting repeated everywhere right.

So, this is called, this is, in this way you can actually capture everything by just looking at one Brillouin zone that is the, that is the beauty of this representation okay. So that is called a reduced zone scheme okay. So, if you capture it this way this becomes a reduced zone scheme, if you only look at the first Brillouin zones. So, if you look at only the first Brillouin zone which I am representing here as writing here as the first BZ.

The reduced zone scheme is representing all the information of the interaction of k vectors, allowed k vectors in the system and allowed the periodicity of the lattice, all represented within the first Brillouin zone. So simply looking at, if I just do this diagram only between these two lines and ignored everything that was on either side of those two lines, essentially, I am only showing you the information within the first Brillouin zone.

It captures all the details of the system perfectly fine okay. So therefore, this representation which is called the reduced zone scheme representation is also good enough for us. So, in many books sometimes you will only see this first Brillouin zone picture shown to you and now you can understand from where that information is coming from. Sometimes they will show you the extended zone scheme.

So, you will see it based on one origin spread out across the entire structure, sometimes they will show you the repeated zone scheme in which case you will see this entire picture the way I have drawn it or ordinarily they are simply show you the first Brillouin zone and you need to understand that it has been pulled together into the first Brillouin zone simply because of the periodicity of the lattice.

What another way of describing it is, you can move every information from every location back by a valid reciprocal lattice vector and it will bring you back into the first Brillouin zone. And that is how you can think of this diagram being pushed back into the first Brillouin zone, if you want. So that is the third way of representing it all three are perfectly fine you can use them based on your convenience and circumstances you can use them.

In this I will also, I also wish to add that we have only shown the E versus k relationship right. The other information that we have not shown here is where is the Fermi energy. These are all the values of E versus k that are permitted in the system in depending on the particular atomic system that you have chosen, the particular material you have chosen, the Fermi energy may be at some particular value okay.

So, I will arbitrarily say that the Fermi energy is, this is the energy scale I will just say that the Fermi energy is here, this is just an arbitrary thing. So, I, you just have to recognise that along the energy axis this plot represent all, represents all the possibilities given this structure and given the values of k vectors that could exist within the structure. The Fermi energy simply depends on what is the number of free electrons per unit volume.

How many is the, what is the density of available states, density of occupied States etcetera right. So, some Fermi energy value is there. Now this Fermi energy value then therefore represents the highest energy level that the electrons can have in the system. So, this can be simply represented here, so you see now how the structure and its interaction with the wave vectors create this band structure here.

The periodic periodic structure of the material plus the wave vectors allowed create this band structure. And within this band structure you can identify the Fermi energy based on where this Fermi energy appears. We are now able to say whether it is a metal it is a semiconductor or an insulator. If it shows up here like the way I have just shown here where it appears in the middle of a band then it the system is called metallic.

Metallic systems are once, where the, you have a half-filled band. So therefore, the electrons are very easily able to move because they are able to see just immediately above them there are empty locations they are able to freely move. On the other hand, you could have had a Fermi energy which finished off at just at the top of this band. In that case we would look at the band gap ahead of it.

If the band gap is of the order of two electron volts or less then that is a semiconductor if we solve the order of four electron volts or higher we would call it an insulator. So, then we will

look at the band gap, we will look at this discussion when we talk of semiconductors we will see that discussion in greater detail. So, this is all the information that we have seen. So, in fact the, it is of interest to see in terms of the material property.

The position of the Fermi energy with respect to these bands is a very important piece of information okay. So that is what we are able to conclude from this one dimensional, detail look at the one-dimensional structure. I will very briefly show you a two-dimensional structure and I will also show you the three-dimensional structure very briefly. So that you get a sense of how the same information is represented in two dimensions in three dimensions.

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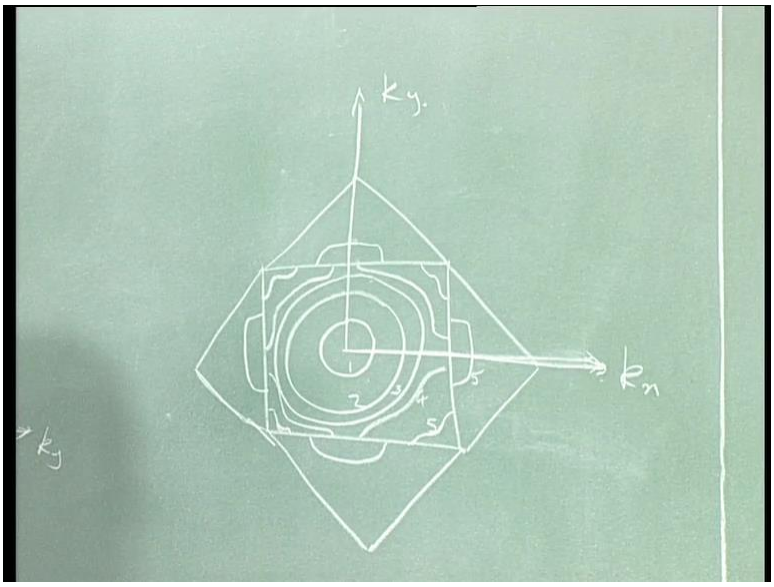

So, we have already seen that E versus k relationship is E equals h bar square k square by 2m, this means in two dimensions, we already saw that in two dimensions a points of same energy are represented as a circle right. That is why it is E equals h bar square k square by 2m in two dimensions, if you write the, if you identify all the points that contains the same amount of energy or therefore all the k vectors in k space.

In k space kx, ky, kz in k space all values of energy corresponding to the I mean all values of k corresponding to the same value of energy are is I am sorry in two dimensions it will only be kx and ky, in two dimensions you have a circle and in three dimensions this would become a sphere. So, these are simply the two cases that we will very briefly look at. So therefore, in a material if you are interested in what is happening to the Fermi energy.

Then you are interested in the last circle that can be formed using those electrons okay. We finished in one of the previous class, we also looked at two-dimensional square lattice and we found that its representation in reciprocal space is also a square, the first Brillouin zone is a square right. Then the second Brillouin zone becomes looks like that and so on. So, we did this we looked at all the Brillouin zones in in two-dimensional space okay.

So so, these are the Brillouin zones, if you draw it properly this would be the Brillouin zones for a square lattice being represented in a square form. So again, we will assume that this is represented in the k vector dimension. So, this is therefore this the diagram that we get here in, if you assume it is in k space, that is scaled properly so that it is in k space. This diagram comes from the periodicity of the structure from the crystal structure.

Therefore, once you once you have a crystal structure this is fixed, you have no choice on this okay. So, this is fixed, however the number of free electrons available in the system may vary depending on the atom okay or even within the, even for the same atom it may have, it may depict a couple of different valences. So, the number of free electrons you have in the system could change.

Therefore, the highest set of energy values that can be attained can differ based on the or rather the Fermi energy that the system might have, which will directly depend on the density of available states and the number of free electrons of a per unit volume that can change. If you assume everything is the same and the density of available states is the same and you are simply changing the number of free electrons per unit volume.

The circle that you can obtain can differ from material to material. So, if you have a material which has a very small number of free electrons you simply have a circle that is like this in which case this represents the Fermi surface, so this is k space, so I will just say this is kx and ky. And we say that, you know the this circle does not interact with the first Brillouin zone okay.

So, everything is within one band, if the number of free electrons is going up it becomes a larger circle, it starts getting close to the boundary of the Brillouin, the Brillouin zone. You can have one more like this, if it becomes even larger what you will see is, it will start distorting, it will no

longer become a circle, close to the circle it will distort like this. So, this is how the Fermi surface now interacts with the Brillouin zone.

And distorts, it is simply an extension of what we saw in the two in the one-dimensional case where we looked at it in one dimensions and we found that it the k values began to distort. And if you go even further you will see that the Brillouin, the behaviour is something like this and it begins to appear in the next zone. So, you can, if you go and look up you will find diagrams like this, where basically so this is case 1, this is case 2 this is 3 this is 4 and this is 5.

And this is 5 these are not the numbers are simply to indicate which curve adds up to which or connects up with which. So, these are all the case where the Fermi surface is just about touching the Brillouin zone and then finally it begins to go into the second Brillouin zone. Again, we can do a reduced zone scheme representation where we basically move things in and represent it. So, you will actually see this as appearing on the side.

This will appear on this side that will appear on this side and so on. So, if you wanted to represent the second Brillouin zone in the within the first Brillouin zone in the above case it will simply look like this, in case four. So, this is how you do this in two dimensions again the diagrams can get complicated if you look at the more and more I mean if you make it a longer diagram and you include all the subsequent zones.

And you continue to grow this I mean and you look at different materials where the Fermi surface is larger and larger and you have to look at interactions between the Fermi surface and much larger and higher Brillouin zones but the concept is exactly the same. You have now got a very good idea of the concept in 1d and 2d okay. So that is exactly the same I will just finish off with a couple of minutes.

Where we look at some slides where we are looking at the exact same interaction the way I have shown you here in three dimensions okay. So, we will do that.

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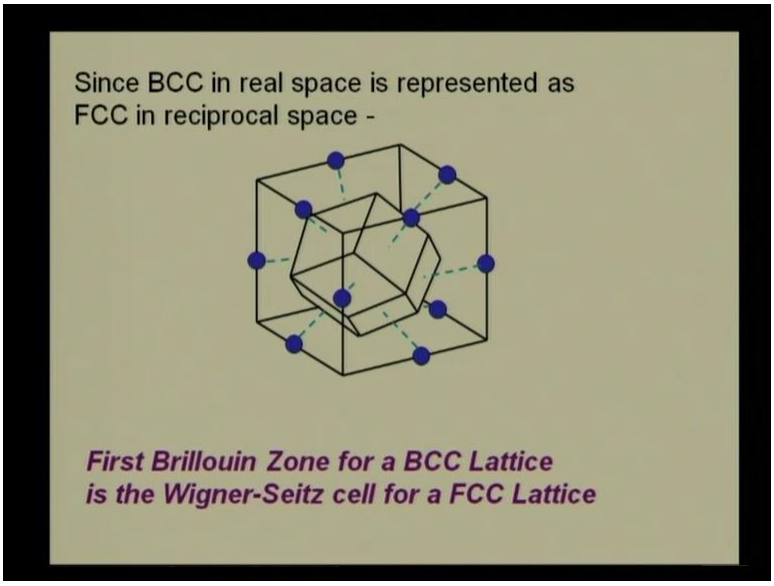

So, we will see now, we saw that we have to now look at first of all the Brillouin zones itself and so we saw already that for a BCC, a material that is BCC in real space it is represented as FCC in reciprocal space and this is then the Brillouin zone okay, so of the first Brillouin zone of the BCC structure in real space which is now represented as FCC in the reciprocal space.

Similarly, we saw that something that is FCC in real space is now represented as BCC in reciprocal space and this therefore the ends up being the Brillouin zone corresponding to that structure. So therefore, now we will see here what, with this structure we will assume that this is the case we are dealing with. It is a face centered a material that is face centered cubic in real space which has been represented as BCC in reciprocal space.

Within the structure we will put in the Fermi sphere okay. Now it is similar it is the same thing it is E equals h bar square k square by 2m and therefore all values of energy corresponding to I mean all values of k corresponding to the same energy are represented by a sphere. So, Fermi surface is a sphere in k space here okay. So, we will look at various possible Fermi surfaces within this which simply represent different materials having the same structure but different number of free electrons per unit volume.

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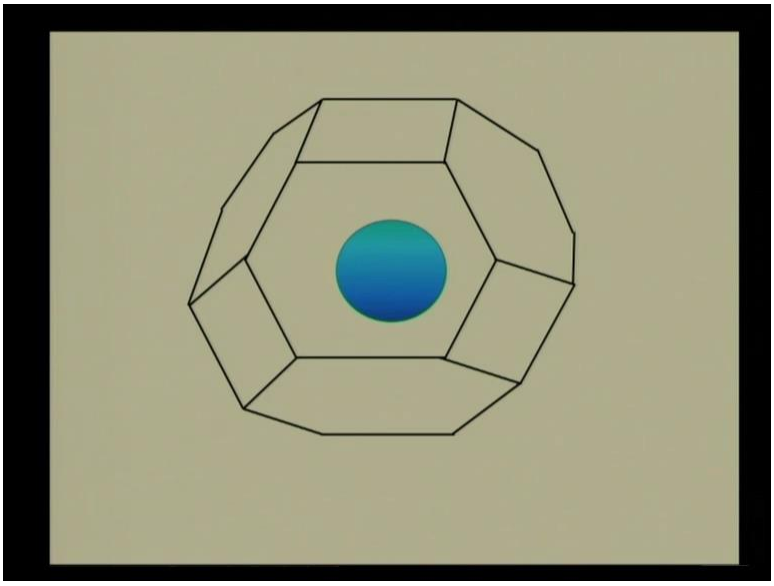

So here is a case where you have a large Brillouin zone and a Fermi sphere which is right in the middle which is kind of small because the number of the electrons is less, let us say okay. We will look at another material, series of materials where the Fermi surface is getting to be larger and larger till it begins to interact with the Brillouin zone and we will just see how that looks. This is a slightly larger Fermi surface still no interaction with the Brillouin zone.

Even larger still no interaction with Brillouin zone, even larger getting very close to the Brillouin zone but not yet any interaction with the Brillouin zone and finally you have a situation where it has gotten very close to the surface of the Brillouin zone these locations of the sphere are getting very close.

This location, this location and this location and correspondingly the other side we are not seeing we are seeing only one side of the figure, these are regions including this front surface, where it has gotten very close to the surface of the Brillouin zone and therefore the sphere is now distorted into this shape, it is spherical up to this point.

Then distorts and touches the Fermi surface and again distorts here, similarly comes here distorts here and so on and similarly distort here. So that is the same way in which we have already seen this in one dimension and two dimensions and I am now showed you in three dimensions. So, to end up to summarize in this class we have looked in detail at the interaction between the various energy levels allowed in the system and the periodicity of the structure.

We have looked at the allowed k values and we allowed the crystal lattice information. We have looked at their interaction and we have seen how Brillouin zones result in, this interaction results in the band structure that evolves for the material and based on where the Fermi energy is with respect to the band structure you see various properties of the material.