Introduction to Reciprocal Space
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Lecture –09
Worked Examples
1. WIGNER SEITZ CELL
2. BAND STRUCTURE

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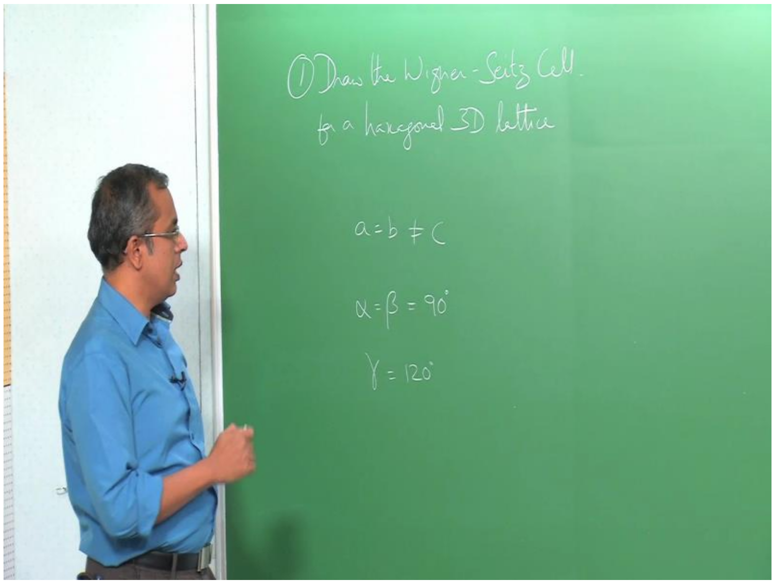

Hello so today, in today's class we are going to look at two worked examples, one will relate to Wigner Seitz cells and the second one will relate to the band structure associated with a 1d lattice okay. So, we do that, so the first question we will try to answer is to draw the Wigner Seitz cell for a hexagonal lattice, hexagonal three-dimensional lattice. So, we will do this as our first worked example.

This you know topic tends to require you to have a visual perception of what you are dealing with and that is the reason why through the classes as well as through this worked example I am looking at diagrams because I think that if you get familiar with the diagrams you start becoming more comfortable with that concept. So, if you take a hexagonal 3d lattice the way it is defined is simply a = b not equal to c with a, b and c being the three axis.

And then the corresponding angles are alpha equals beta equals 90 degrees and then gamma equals 120 degrees. So of course, when you draw diagrams the, we tend to be more comfortable with cubic systems to draw. So that is specifically why I have chosen the hexagonal system to see if we can, you know make ourselves comfortable with the hexagonal system as well and therefore we will do this example.

And of course, as I said here you know alpha equals beta equals 90, so gamma is not equal to them not equal to alpha and beta is equal to 120 degrees. So, we will first draw this unit cell, so what we will find is this unit cell as such is drawn will not give us enough scope to complete drawing the Wigner Seitz cell. So, we will actually have to add more pieces of this unit cell and build a structure. In that larger structure, we will have a central lattice point around which we can draw the Wigner Seitz cell okay. So that is what we will do.

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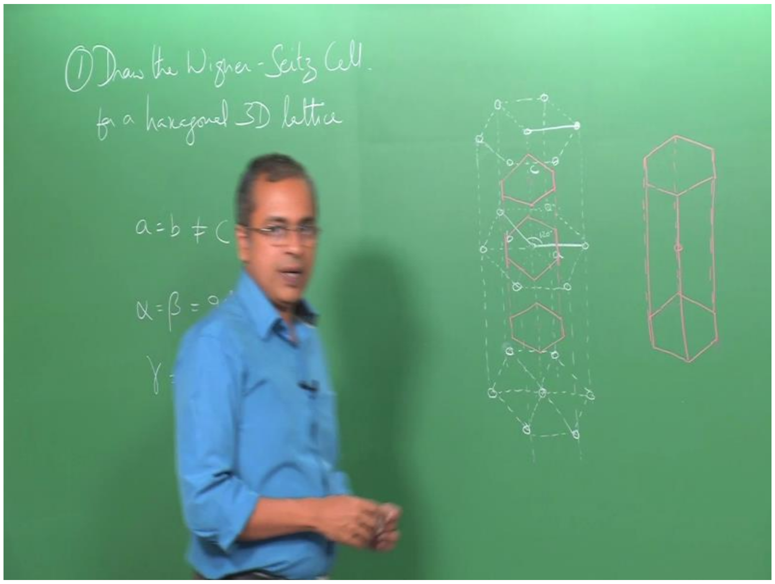

So, if you see here we will just basically take a point here and a point here and then we will just consider the point here. So, we will say that this is 120 degrees, so that is your gamma and then we will draw the rest of this unit cell. So, the, if I just draw a parallel line here so somewhere here is where I would get the other lattice point.

Then I can draw that here, a little bit more this way okay. So that is three of them and four of them and then we can just take this up, so you we just complete this diagram here, so that is your unit cell for the hexagonal system. So, this would be based on what we just put down, this we can designate as a, this we can designate as b, this axis here would be your c axis or in this case this would be the c axis here a to bc and so that would be your a b and c axis.

The gamma angle is opposite the c axis, so that would be that 120 degrees that use, that you see there and alpha and beta would be 90 degrees, so this is what we have. So, as it turns out no this is not sufficient for us to complete drawing the Wigner Seitz cell, so we actually need to have one central lattice point around which we are going to draw the Wigner Seitz cell.

So, we will actually choose this to be our central lattice point, so we have actually draw enough unit cells around it. So that we can get the other lattice points around which we can know complete this diagram. So, if you just take the central hexagon here and also you must notice that you know when you see the shape as it is drawn on the screen it does not immediately look anything like a hexagon but we have been calling this hexagonal lattice.

So actually, when we put in some more of these unit cells around you will begin to see the lattice structure that we are looking at which we would call hexagonal, so we will just do that. We will add a lattice point here which would be the next status point that would come here it will be diametrically opposite to this, so you will get a point here, you can extend this and diametrically opposite to that, you will get a opposite to this point.

You will sort of get up point here that would be a lattice point and extend this here and you will get a point here and we can continue building this unit cell. So, if I now complete this structure you begin to see the hexagon, so you know see a hexagon and this is the base of one of those unit cells, this is the base of another unit cell, this is the base of a third unit cell. So actually, there are three unit cells the base of three unit cells is here, it is not all of the cell is not here.

The base of 3 unit cells is here, so I will just do the same thing for the top lattice, so that we can complete the diagram but even that will not be sufficient we will need to draw one more below it which we will do shortly. And then we would need diametrically opposite to that, which would be somewhere here, diametrically opposite to this would be somewhere here. So, we can complete this diagram.

So that is the hexagon on top, that is the hexagon at the bottom right now, we need to actually generate a hexagon below as well, so we will just do that and with that we will have enough points on the board that we can draw the Wigner Seitz cell. An equal distance down here, so that would some put it somewhere around here, so we have a point down there and then we just go across get a point here.

We got ourselves a point there and two more points and two more points on either side. So, we can just continue to this down here and we basically have a point here roughly and a point roughly there and similarly you can extend this further down, down there. And you would have a point roughly here, so actually this would have to be little higher and you would have a point down here and therefore you get your hexagons somewhere here okay.

So those, that is your hexagon okay, so we have actually, you know what this hexagons put up here. So now we would like to draw the Wigner Seitz cell, so we have enough points here that we can construct our Wigner Seitz cell, so that is why we needed to make this diagram a little bit more elaborate. So, there is a hexagon in the middle, like hexagon on top, hexagon at the bottom.

And then we have the lines connecting those respective points and that is how we have got the overall diagram. Now we will treat this as our central point, so around this we can actually draw our Wigner Seitz cell. So, as you can imagine we need to draw the perpendicular bisector of the lines joining this central point to all its neighbours. So, there is a neighbour here, so the perpendicular bisector would be somewhere here right.

So that is the perpendicular bisector, this is the neighbour here, so that is a perpendicular bisector here. There is a neighbour there, so that is the perpendicular bisector to that, perpendicular bisector here, this is neighbour here, so you get a perpendicular bisector to that and so on. So, a one more neighbour here perpendicular bisector to that and you would get one more here, so you would actually get a hexagon that looks like that okay.

So similarly, you would get one below and one above but basically, we do not need to go all the way to the bottom and the top, we as you as I mentioned the Wigner Seitz cell is bounded by all those perpendicular bisectors that connect, that bisect the lines connecting that central point whatever is its nearest neighbour. So, the nearest neighbour on the top direction is this point and similarly the nearest neighbour the bottom direction is this point.

So, we need to bisect halfway here and halfway there, so you will have hexagons here at the halfway mark, so roughly if you take this as the halfway point, we have to build an identical hexagon here, so you will get something like that and this would be a hexagon about this point. Which is actually not a lattice point but it is at that plane actually. It is in that plane and similarly you will get a hexagon here which is roughly at the halfway mark here.

And you would basically see as hexagon that looks like that okay. So, these are actually at an incline, so I mean this is hand drawn figure but this is this one lattice point here, this is the midway plane here, this is the midway plane here. So actually, if you connect this up, this is then you are Wigner Seitz cell about this lattice point. So just for clarity sake I just draw it roughly at the same position here, so that it is clear and you would have a hexagon down here.

These are regular hexagons they are just at an incline to us, they are inclined to us that is why they do not look like regular hexagons where you see them here and we can connect this up, that will connect up there and you want that connect up there, this would go up to the front, connect up to the back right. So, this hexagonal prism whatever I see here is what I have transported here this is a hexagonal prism, this hexagonal prism is the Wigner Seitz cell for the hexagonal lattice.

So normally you know it is a little bit you know we get a little vary if you have to draw this for a structure that is not cubic but it is really not that difficult if you actually look at this diagram and I have just drawn it here, central point, this is a hexagon below a hexagon above of lattice points and then there is a middle mid level plane, a mid level plane that bisects the line joining this point at this point.

There are no, there are no lattice points at this plane at this point, in this diagram also no lattice points of this plane, only a central lattice point. So, if within, so this prism will essentially be the central point that lattice point would be sitting here and then that would be the Wigner Seitz cell for the hexagonal lattice. So that is the answer, we have solved this example here too look at the Wigner Seitz cell for a hexagonal lattice. So that concludes our first worked example.

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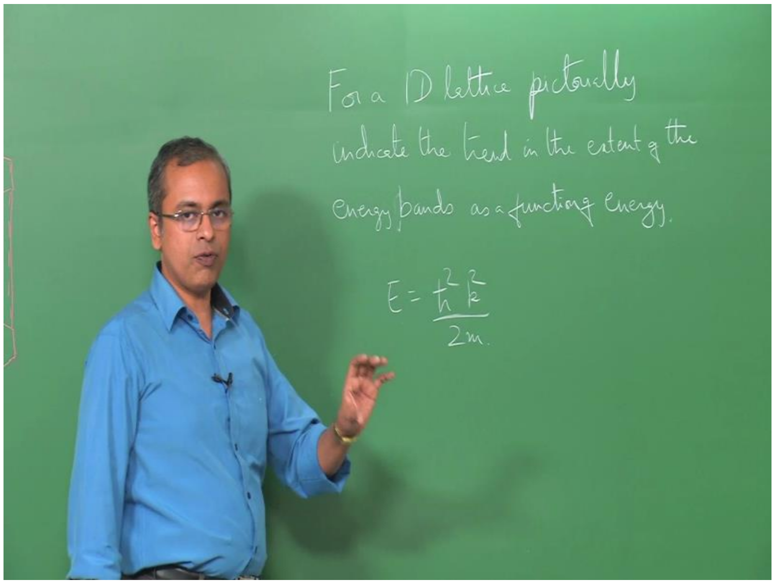

We will now look at another worked example which is for a 1d, lattice pictorially indicate the trend in the extent of the energy bands as a function of energy. So, we are basically looking at a 1d lattice, we would like to pictorially indicate the trend in the extent of the energy band as a function of energy.

So that is basically what we want to do, we have actually drawn E versus k diagrams for this, so we have E equals h bar square k square by 2m and it is on this E versus k diagram that we also draw the Brillouin zones of the 1d lattice and on that on the basis of those two diagrams is what we come up with the band's. So that is the diagram that I am going to draw and I am going to show you that the bands are not of uniform size but they keep varying with size with energy.

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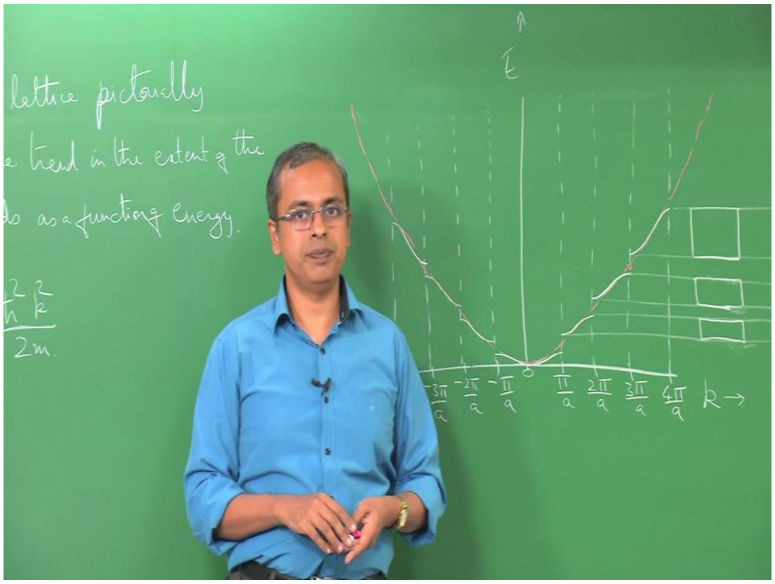

So if you look at it here, we draw this diagram here, we have E here, we have k here and that this is the origin we have Brillouin zone boundaries at intervals of pi by a, so pi by a, 2pi by a, 3pi by a and 4pi by a, I just pick for four such boundaries and similarly we come back here we have -pi by a or pi over a if you prefer to call it that -2pi over a, -3pi over a, and -4pi over a, so that is a matter of usage some people say pi by a, and some will say pi over a.

But anyway, that is the idea that we are trying to convey. So, this is k, k vector this is energy heading that side and the, so the Brillouin zone boundaries are here, so we just draw the Brillouin zone boundaries. On this diagram if we draw the E versus k a relationship for a nearly free electron, you are going to get a parabola because it is E equals h bar square k square by 2m. So, we will just draw the nearly free electron parabola that and that would be something like that.

So, something like that, so I just darken that, so that is the E versus k a parabola just a hand drawn diagram of it and so from this the band structure comes and as we saw it comes something like this. At the Brillouin zone boundaries, there is a distortion of the E versus k relationship, so it becomes like this and so we have similar drawings diagrams here. And so, from this the band structure comes, so if we draw the band structure here this would be a band.

So, this would be a band, this would be the next and this would be the band above it. So, the question is what is the trend in the extent of these bands as a function of energy? So, energy is going up, what is the trend in the extent of the bands as a function of energy, so as you can see as the energy goes up the band, the extent of the band actually keeps increasing. So, you have a smaller band a little larger band and even larger band as you go up.

So, as you go up in energy the extent of the band increases, so that is the basic answer. The reason for it is quite straightforward that is because the Brillouin zones are linearly spaced. They are spaced as pi by a, 2pi by a, 3pi by a, 4pi by a and so on, so there is that spacing is linear. Whereas the E versus k relationship is parabolic, so this is this relationship is parabolic.

This relationship is linear and as a result of those two you find this trend in at this for one dimensional lattice you can see that trend here that the band structure is such that the bands are narrower as at lower levels of E and as you go to higher and higher levels of they become wider and wider okay. So that is the point that I wanted to make with this worked example.

So, we have seen two worked examples one relates to the Wigner Seitz cell for hexagonal three-dimensional hexagonal lattice and the other relates to the band structure of a one-dimensional lattice okay. So, with that we will halt today. Thank you.