**Electronic Theory of Solids**
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**Lecture - 16**
**Brillouin Zones**

Hello. We have been doing calculations on determining the band structure of electrons. This involves basically again a single picture in quantum mechanics where we try to understand the solution for an electron for a single electron for example, in a potential from the ions which; obviously, has the symmetry of the crystal.

So, the ions the atoms form a Bravais lattice in a and that Bravais lattice we define what is a Bravais lattice. Basically, set of points in regular arrangement and orientation each of these points must be must view the lattice exactly the same way from any other point. So, and that Bravais lattice generally that is the Bravais lattice is generated by a vector R which we defined previous day.

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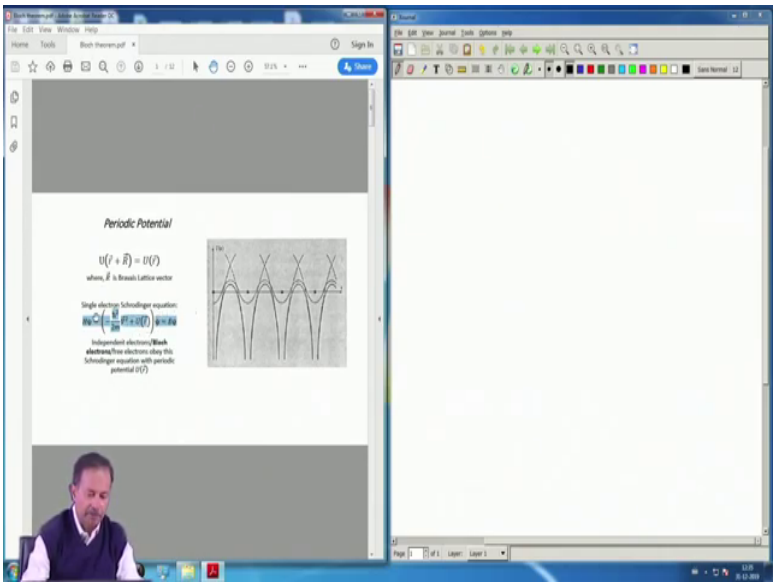


And, in the previous class and what we said is that the potential therefore, has this periodicity a potential U which is which has the periodicity of the Bravais lattice. And, this is a 1

dimensional rendition of this periodicity for example, the ionic potentials or sort of diverges towards minus infinity its Coulomb potential.

So, at R equal to at every location of the ion the Coulomb potential goes to almost minus infinity. Although, in real solid it will never go to minus infinity and there are other effects that will cut it off, but it becomes very large at every ionic site and then very quickly dice down away from the site.

So, this is the periodic potential in which the electron is moving. The assumption is that the electron-electron interaction between electrons is negligible as well as the fact that the dynamics of the nuclear the atoms is completely neglected.

And, this the second is called the Born-Oppenheimer approximation and the fact that we are ignoring electron-electron interaction means we are still in the independent electron approximation. So, under these approximations we embark on solving these Schrodinger equation for a single electron in such a periodic potential ok.

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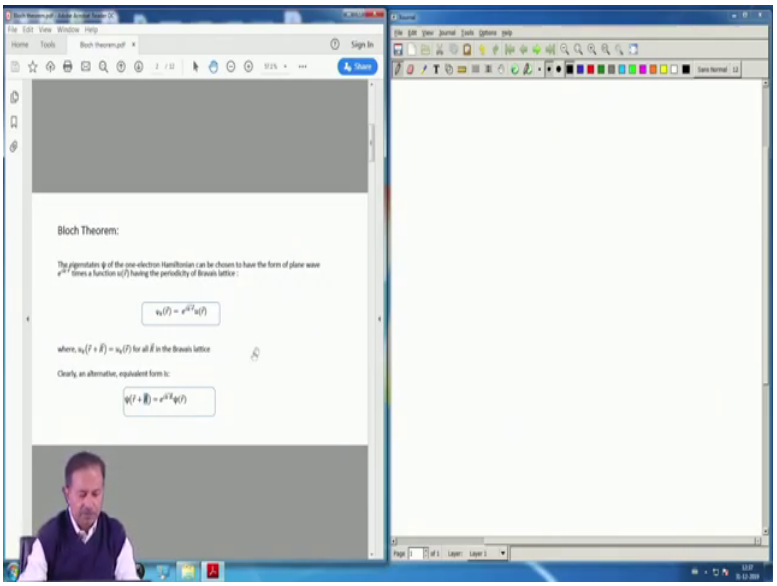


So, and we mentioned that there is this very well known theorem which was written down by Felix block where what we showed is that the wave function must have this kind of a form psi k of r is e to the power i k dot r u of r, where u can also depend on k.

So, this u k of r plus capital R is p is the same as u k of R, that is this u functions small u function carries the periodicity of the Bravais lattice on which we are seeking a solution. Now of course, this leads to the corollary clearly that psi of r plus capital R is just phase factor time is psi of k of r.

So, psi k r plus capital R is e to the power i k dot r psi k of r and this is trivial you can just add a psi r plus r here and this term will give you the first phase factor will give you e to the power i k dot r and the second one being periodic will remain the same. So, that is the phase factor that you can you see this is very powerful in the sense that this tells you that if you know the solution at any unit cell point r then you know the solution at any other unit cell point.

Any other point inside the unit cell which is far away from it anywhere in the lattice actually by just translating by this Bravais lattice vector. So, that is the; that is the very powerful theorem and this theorem basically narrows down the class of solutions that are admissible for an electron moving in a periodic potential ok.

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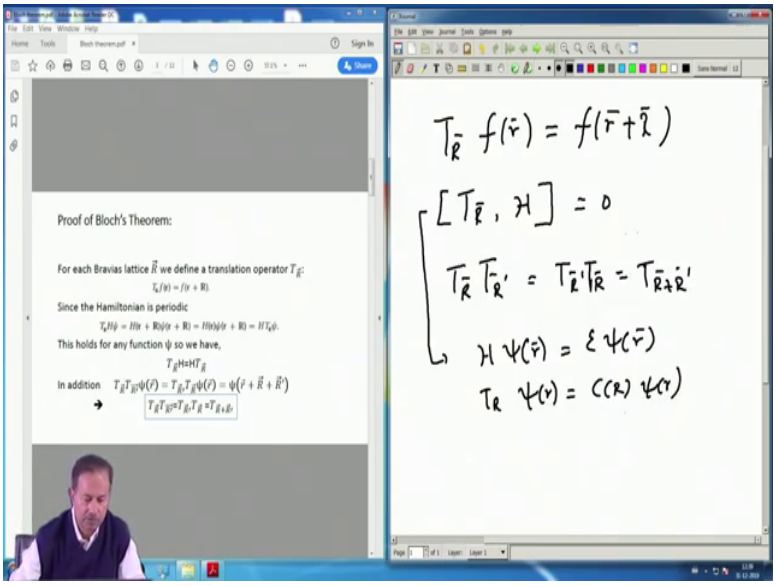


So, then of course, we came to this so, called proof not a derivation, but a proof of Bloch's theorem which shows that is exactly the form that during functions must have. So, it starts with this translation operator a translation by a Bravais lattice vector capital R. So, that

translation vector translates any function; so, that we said is that it translates any function T of R operating on any function r we generate f of r plus R.

And, then we found out certain properties of this R and one of them is this one that T of R commutes with the Hamiltonian. This is a very interesting property because this commutation allows us to use a very fundamental theorem in quantum mechanics which says that, if you have; if you have two commuting operators or a set of commuting operator then you can have a simultaneous wave function. So, you can choose a wave function which is a simultaneous wave function of both of these.

In addition we also found that this T of R has this property T of R and T of R prime is they again commute T of R prime T of R and this is the same as T of R plus R prime. So, this property then so, this then allows us to write H psi of r equal to E psi of r and simultaneously T R of psi of r equal to some c of R psi of r.

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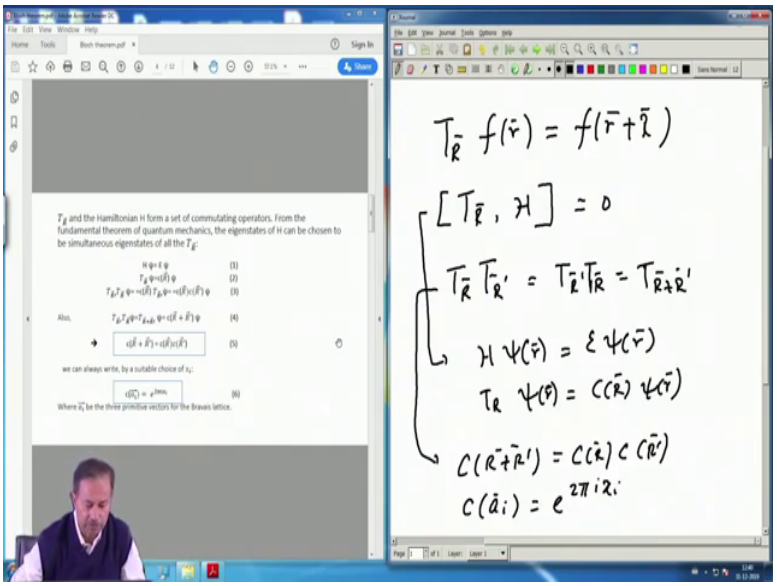


So, we will use these properties to determine the admissible solutions for psi of r and that is what we did that this property for example, immediately implies that c of R plus R prime is equal to c of R into c of R prime ok. And then of course, we can then write that c of a i any Bravais lattice vector a primitive lattice vector is equal to e to the power 2 pi i x of i where we showed that x of i has the form that writing.

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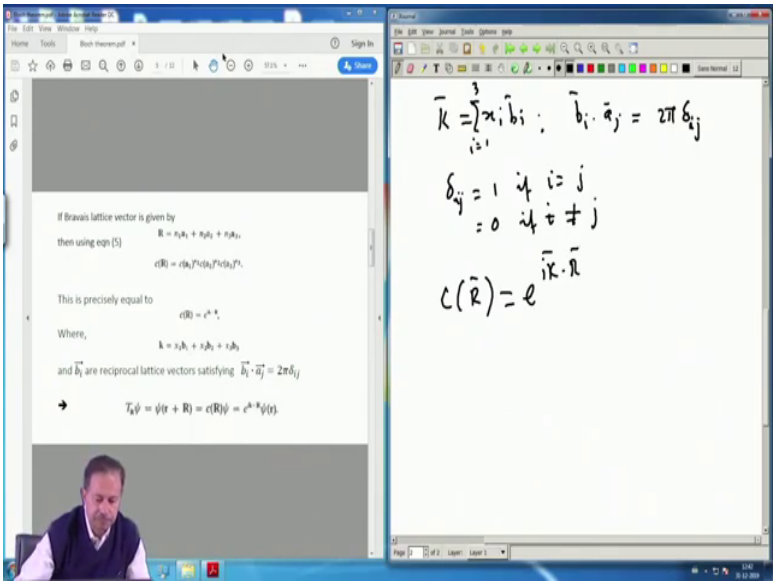


Then we can what we can do is that we write vector k k equal to x i b i sum over i equal to 1 to 3. And, in 3 dimension and where it satisfied this relation b i dot a j equal to 2 pi times delta i j, delta i j is the chronic or delta symbol. So, where delta i you remember delta i j is 1 if i equal to j equal to 0 if i naught equal to j. So, that is the so, that that basically says that if a i is are primitive lattice vectors in the real lattice then b i's are the reciprocal lattice vectors, that is how reciprocal lattice vectors are defined.

So, therefore, c of R can be chosen at as e to the power c of R can be written as equal to e to the power i k dot R. So, this is the this is my k vectors, these are my reciprocal lattice vector. So, k is a vector in the reciprocal lattice.

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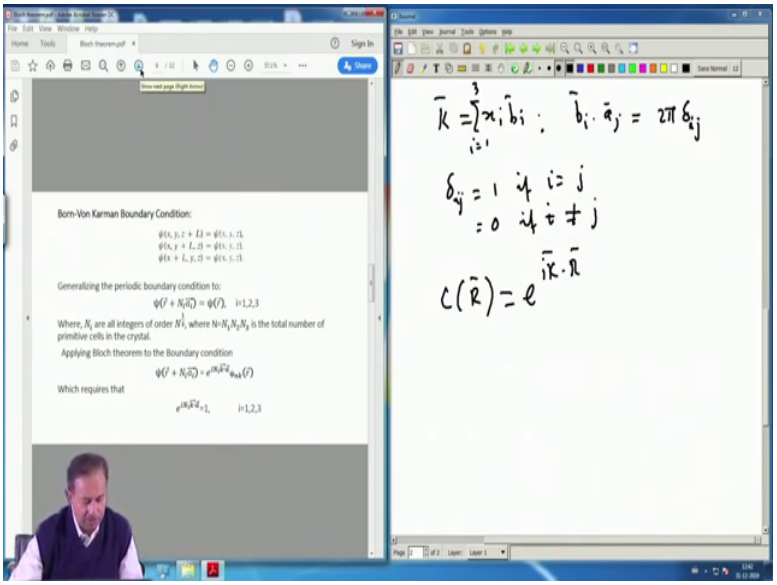


So, what we did next is that we basically showed that Born-Von Karman boundary condition can be applied here also and that gives me the values of k that are.

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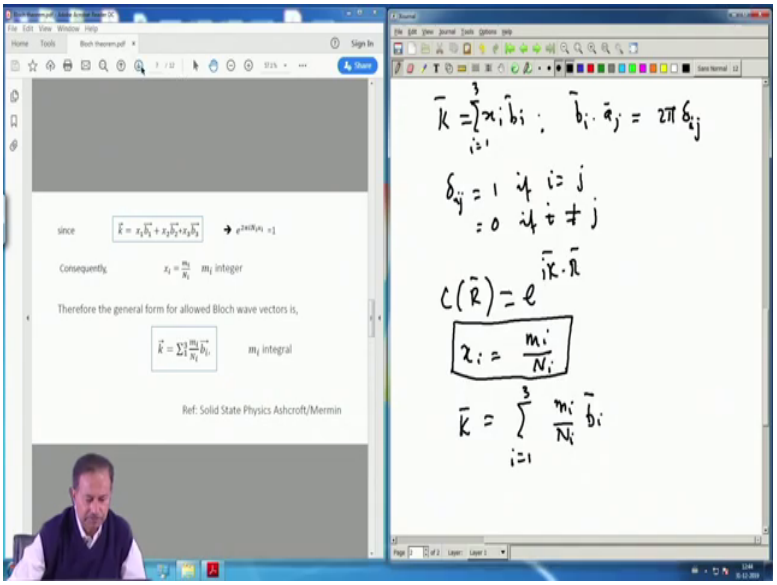


So, values of k means values of x i; so, then one found that x i will be some integer m i divided by the direction the size of the number of lattice sites in the direction or number of

primitive cells in the direction of i. So, that is the these are technicalities I mean its basically tells you that x x i has to be written in this way and therefore, k has a specific form.

So, i equal to 1 to 3 m i by N i into b i ok; i is i defines the directions along the 3 along a 3 b i directions ok. So these so, this completes the sort of showing that Bloch's theorem holds sort of a its a proof of Bloch theorem that the any electron moving in a periodic potential; if you solve its time and dependent Schrodinger equation then you will get a solution whose form is in this the form obeys the Bloch's theorem. So, that solution we obey Bloch's theorem with; so then.

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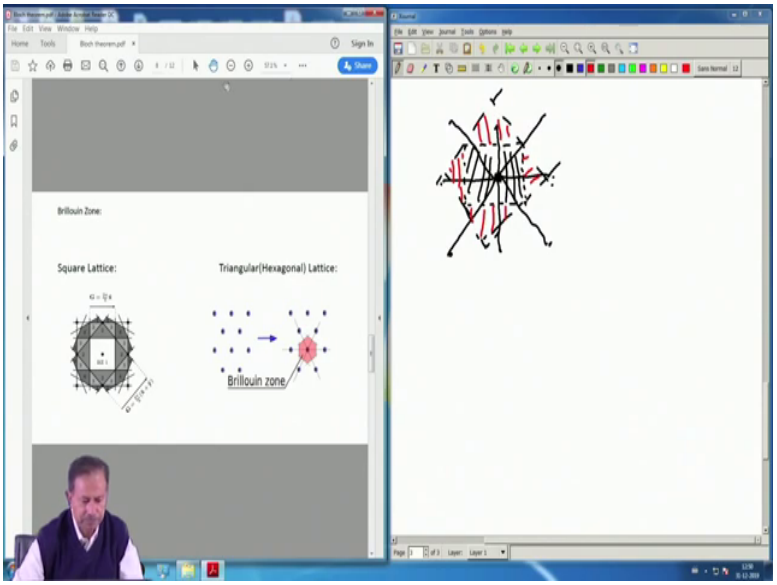


So, let me just show you for clarity how these things work in reciprocal space. In the reciprocal space for example, one defined something called a Brillouin zone, this probably you have done in your elementary condensed matter course. The Brillouin zone is basically the is called the Wigner Seitz cell in the primitive lattice.

What it means is that you take a any Wigner Seitz cell in the reciprocal lattice. So, take any point in your reciprocal lattice then what you will do is that to find what is the Wigner Seitz cell the procedure is very simple, just join that point with all is nearest neighbors. So, for example, let me show you suppose you have a square reciprocal lattice is a square.

So, this is a point it has all the; so, this just look at this point. It has 4 points on its 4 sides. Now, to get the Brillouin zone all you do is to connect this point to all its nearest neighbors and then draw a perpendicular at the middle of all these lines.

And, then the area covered by all these 4 perpendiculars that defines an area which is closer any area inside this dash square for example, is closer to this point, this point central point then to any of its neighbors ok. So, this region this region is therefore, the Brillouin zone of this lattice reciprocal in the reciprocal lattice; so, that is how it is constructed.

So, this is you can go on constructing it by connecting to. So, this is the first Brillouin zone, you can do the same for the next nearest neighbors which are here. You can join these and then draw perpendicular. And, this region for example, this region its outside the first Brillouin zone and within this a new square is your second Brillouin zone and so on.

You can go on doing it which is what is shown in this a for a square lattice for example here. So, this is Brillouin zone number 1, then Brillouin zone number 2 and Brillouin zone number 2 is here as I just drawn here in my in this on the right hand side, the red dashed region and so on. I mean you can go on doing this procedure ad infinitum.

The advantage of doing this is that the that is something may have already done, but I have already know may already know that there is a you can define your energy spectrum within just Brillouin zone. And, then it is you can just repeat the you can rid of the energy of any other zone of the solid by just translating by a reciprocal lattice vector.

So, because the energy is invariant under the translation of a reciprocal lattice vector the necessary is to the we only need to know the energy in only one zone which is the first Brillouin zone normally taken.

But, this is not necessary it is a very useful scheme to write down the energies of energy spectrum of a regular solid Bravais lattice for example. And, it helps us that we do not have to know the energy for every k, all you need to know is the energy spectrum within the first Brillouin zone then you know the energy spectrum anywhere else.

And so, let me show you how it is done. So, this is for example, the right hand picture is the Brillouin zone for a triangular lattice often called hexagonal lattice also. Do not confuse it

with the honeycomb lattice which is for graphene I showed the other day. This lattice, the honeycomb does not have the central point, this see this is a hexagon, but there is a point at the center.

So, this makes the this is now a triangular lattice or a hexagonal lattice whereas, in honeycomb lattice you will have these hexagonal structure without the central point. So, that is not a Bravais lattice whereas, this one is ok. So, the if you draw the Brillouin zone its drawn here the first Brillouin zone it is a is again a hexagonal the reciprocal lattice is also hexagonal uh.

So, from real lattice you come to reciprocal lattice and in the reciprocal lattice you draw this region which is closest to this point then any other point ok. So, that is the method that is called the Wigner Seitz cell and that is what one does to find the first Brillouin zone and go one can go ahead and do find out the second, third, fourth and so on Brillouin zones. So, this is the zone in which one remains interested for calculation of energies and anything; everywhere else can be, but rid of from this energy spectrum ok.

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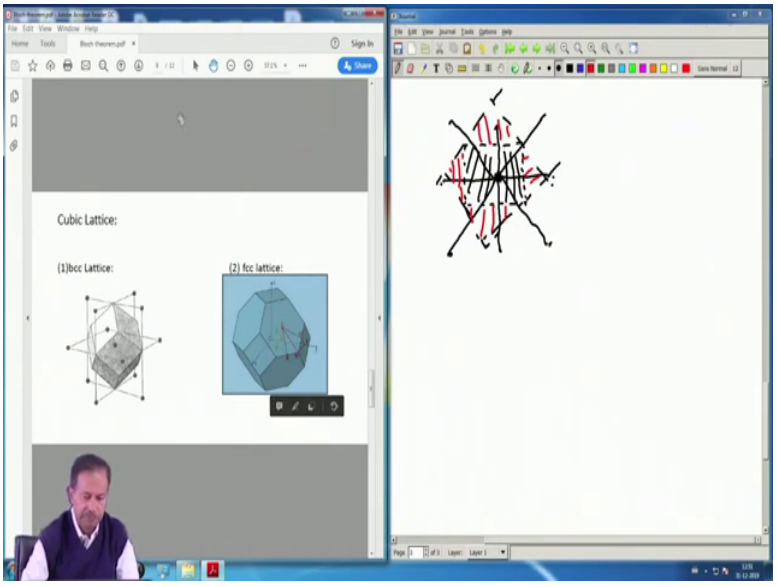


So, these are more complicated one this is for example, in a cubic lattice where this is hard to draw by hand. But, in a cubic lattice you can see that the same scheme has been applied and

this is for the fcc lattice, this is for the bcc lattice. So, see body centered cubic lattice, this is face centered cubic lattice and so on.

One can go on doing the same the procedure is the same instead of lines now you have to draw plains perpendicular to the line joining the central point to its nearest neighbor. And, that is the way it is done, the central point is often called the gamma point.

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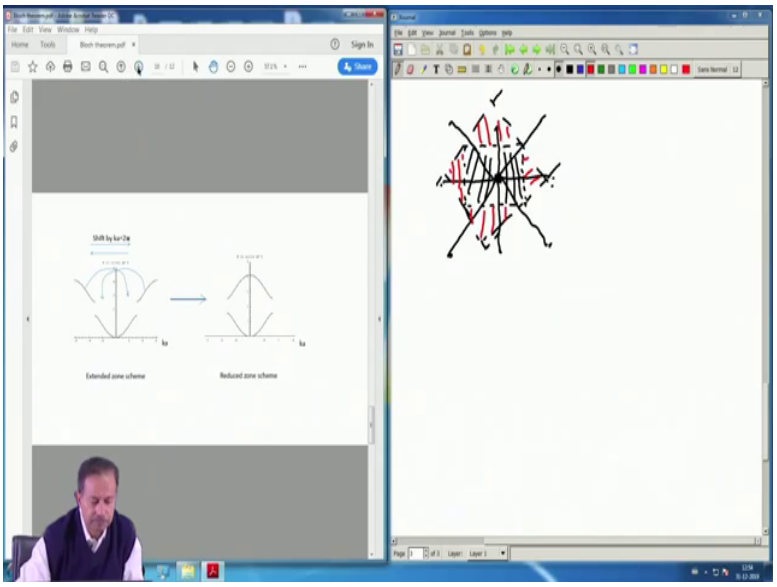

Now, as I said look at for example, in energy spectrum like this with a gap at the zone boundary, if you look at this unit is k a. So, k a equal to pi from pi to minus pi is the first Brillouin zone so, and there is a gap. So, let us not bother about this gap, but suppose we have an energy spectrum which has the structure.

So, then the energy spectrum can be so, this is like the this part of the spectrum is this part and this part. These two parts have gone beyond the first Brillouin zone and then what one can do as I said is that you can translate that by a reciprocal lattice vector which is 2 pi by a 2 pi here k equal to 2 pi.

So, k will be 2 pi by a and if you translate then this left hand part this part will come to the right and the this part this right hand part which is outside of the Brillouin zone will come to

the left. And, they will both go inside the first Brillouin zone and this is exactly what was happened. So, these arrows tell you how to translate it.

So, this one this piece goes here, this piece becomes this piece and this one which is in the second Brillouin zone now goes here becomes this piece, this one this part sorry this part. So, that is called the reduced zone scheme and this is the extended zone scheme. This is the one which we normally draw for all k going to any k pretty large k's also.

We can go on drawing it, but all of these pieces which are outside the first Brillouin zone can be brought to this to the inside the first Brillouin zone by transition translation through a reciprocal lattice vector which here in 1 dimension is k equal to 2 pi so, k equal to 2 pi by a.

So, this scheme is called the reduced zone scheme, most of the band structures that you will find in the literature, in papers are done in this zone scheme. So, they will only consider the first Brillouin zone and plot the band structure in certain directions because in 3 dimension there are many different directions in which you can plot a band. So, people choose certain symmetry directions in the lattice and plot the band structure accordingly in those directions.

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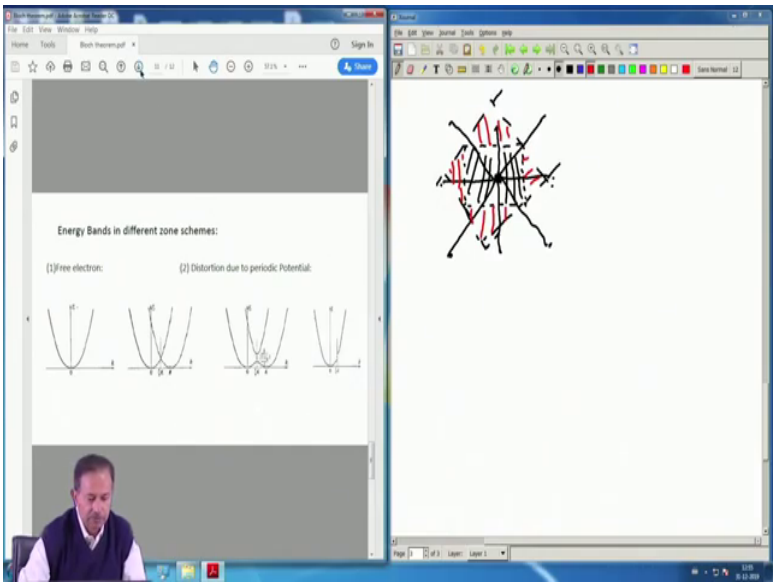

So, this is an example of how to draw energy bands in different zone schemes. And, as you can see that this actually has a periodic potential causes a distortion in the band and that distortion opens a gap here a distortion the; so, distortion due to a periodic potential.

So, periodic potential will change the band and open a gap at the zone boundaries at certain points, here it is a certain point called half k, k is a certain direction in the Brillouin zone and so, symmetry direction. So, there is this example shows that this is this can be drawn in different zone schemes. So, this is basically now it is brought back to the first Brillouin zone.

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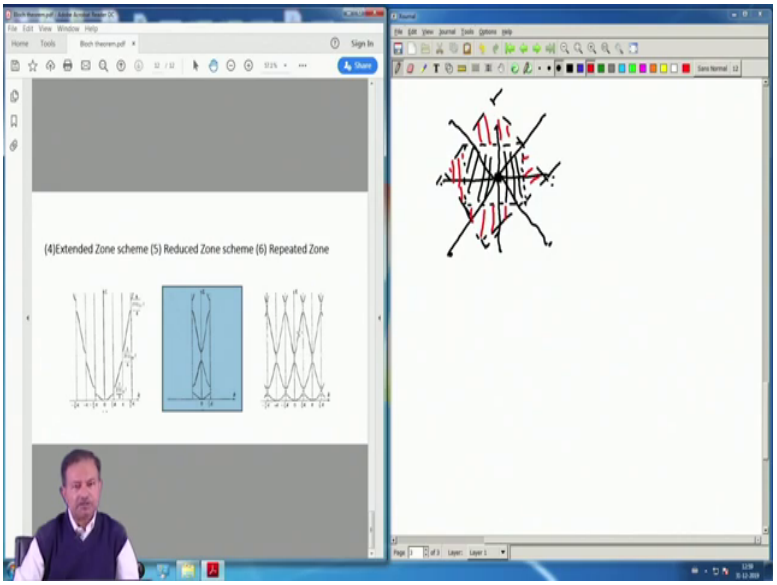


So, here is another example. These first two we have already done, we have already shown how to do it. For example, this region and this region and this region for example, they migrate to here. On the this share this region that one which is highlighted here will go to this to become this band, in the reduce zone scheme.

And, these left hand side will go to the, left hand one we will go to the this one in the first zone. So, we are bringing things out from second Brillouin zone into the first Brillouin zone. Look at this is now in the third Brillouin zone and this will have to be brought into the first Brillouin zone. So, you will translate by two reciprocal lattice vector and this is exactly what you will see, this is how it will work.

So, this can be a brought to this will come here and this the other one this one will come here by a translation of a reciprocal lattice vector. So, one can go on doing this and look at the reduced zone scheme how it looks like, this is the first Brillouin zone. And, and you can repeat the first Brillouin zone, this is called the repeated zone scheme; it is not popular.

The one central one is the one which people mostly use this one, the bringing everything into the first Brillouin zone. And, this is basically repeating it I mean just first Brillouin zone is being repeated on both sides. This one is the one which is the popular choice for doing a band structure calculus, you are showing a band structure.

So, this is how the Bloch theorem help us helps us to find out the nature of solutions, the property that the solution will have. And, the way the solution and gives the ones you find the solution then the solution gives an eigenvalues, you have the eigenvalues.

The eigenvalue will depend on the k vector in reciprocal lattice and that energy basically that is the energy, energy depends on the k value reciprocal lattice vector. This is called crystal momentum k and that the e versus k plot is done on a reduced zone scheme where every energy is the every, the energy is shown in the first Brillouin zone and this is the this is called the reduced zone scheme.

So, everywhere you will see E versus k plot then you will find that it is shown in the first Brillouin zone. And, why can we do it why do we; why do we do it in only one Brillouin zone in the first one? It is because its makes life so much simpler, the rest can all the obtained by just a translation of a reciprocal lattice vector.

So, periodicity of a lattice or a Bravais lattice gives us this enormous freedom that we only need to calculate our find our energies energy spectrum in first Brillouin zone and that is all we need. Similarly, the solution is required to be found only in a primitive unit cell. And, then you can just extend it by you know how to extend it by just a phase factor to find out the wave function in any other region of the lattice. So, just one primitive cell is good enough for you to find out the wave function. Similarly, for energy is just the reduced first Brillouin zone that is enough, beyond that is obtainable from this energy spectrum. So, that is how it all works.