Solid State Physics
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Lecture - 44
Band Theory of Solids (Contd.)

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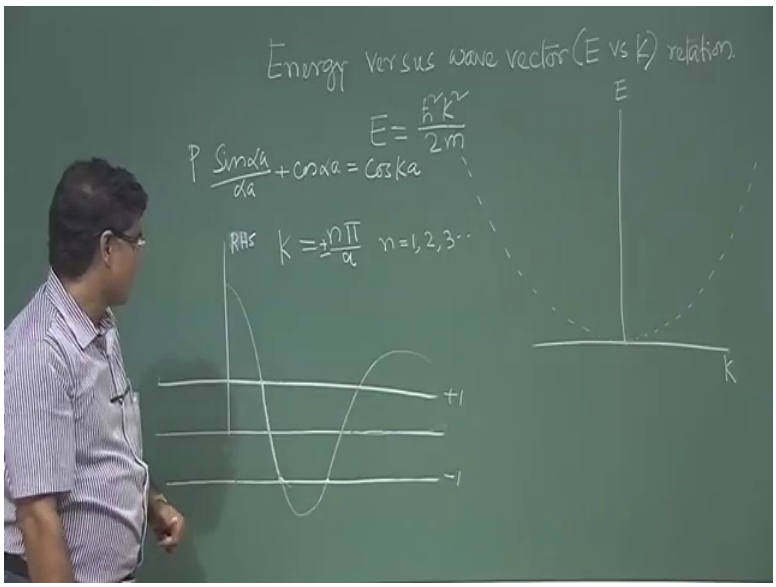

So, we will continue our discussion about the energy versus wave vector that is basically E versus K relation. So, this is very important relation we will see later on, but let us find this relation. So, for free electron this relation we have seen that E equal to h cross square K square by 2 m. So, E is proportional to K square. So, it is let say parabolic relation, see if I plot K, this is E and this is K. So, this E equal to this proportional to K square. So, it will be see parabolic right, for plus minus K value for plus minus K value E will be positive right.

So, this relation between E and K that is for free electron, now in case of periodic potential or the when electron is in a lattice. So, then the relation P sin alpha a by alpha a plus cos alpha a equal to cos K a. So, that relation has to follow. So, now here you can see that right hand side is maximum value can be plus minus 1 so; that means, K can take value N pi by a or plus minus N pi by a where n equal to1 2 3 over or N pi by a then n equal to plus minus1 plus minus 2 plus minus 3 etc.

So, because if you put K here. So, then it will be N pi so, it will be plus 1 or minus 1 for

these value of K; so here this K so from this condition, whatever the K value we are getting. So, this K value so here another point we have to that if I that, if the throughout this right hand left hand side. So, it varies like this right. So, it is value between plus 1 and minus 1 right. So, this value is restricted by this right hand side right. So, this equal to this, so this left hand side whatever it can be right hand side also right, but this right hand side this value only can content between these 2 lines right.

So, here so this and this point if we consider. So, this is the K value we can say this is the K value, this for a particular this is the K value are allowed. So, right hand side if I just between these 2. So, these are giving basically extinct point plus 1 and minus1 for this K value it is giving extreme point plus 1 and minus 1. So, between these 2 So, K value for this K value what about this term I am getting plus 1 and minus1 and all these along this line this is for all K value are allowed, all these K value will satisfy this condition because this value is not only plus 1 and minus 1 in between value, also satisfy this condition. So, here this K as if this continuous K as if this is continuous right, then there is a discontinuity here; again K value starts from here and between these 2 again this K value are allowed this K value will be allowed. So, what does it mean?

So, when electron in a periodic potential in a crystal then, all K value is not allowed like K is continuously increasing here. So, that is not allowed. So, certain range of K value are allowed and then there will be discontinuity, where the discontinuity when K equal to plus minus N pi by a. So, discontinuity for discontinuity will come plus pi by a and minus pi by a ok.

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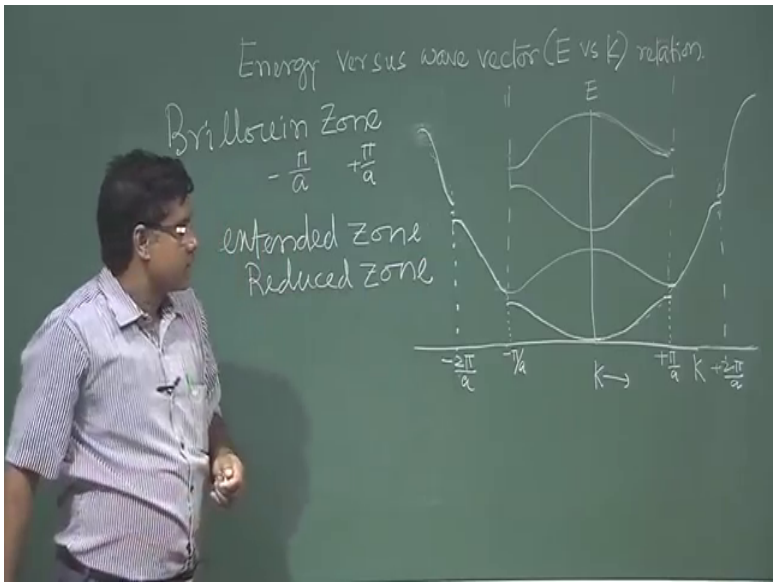

So starting from here, in this case as if this K will vary; so K will vary like this continuously it will vary and then here if it is plus pi by a and it is minus pi by a, then it will be there will be discontinuity at this point and then again it will start to vary for starting from plus K by a to plus 2 pi by a and minus pi by a to minus 2 pi by a. So, as if for this point so this are again this will be allowed. So, this comes with this will be allowed now, so then same K value but it will be different.

So, this it will be continue from here to here. So, this will be minus 2 pi by a and so if I replace. So, this part will be plus 2 pi by a plus 2 pi by a. So, similarly let me continue then you will get. So, this next K will start from here, I think like this. I think I have to yes. So, for this plus 3 pi by a and inside this side this minus 3 pi by a. So, here this what about this for electron it was the curve E and K whatever the relation was there, this variation was there, but when the free electron is in crystal is in periodic lattice. So, this no longer that is relation is the valid, this relation will be different between E and K and that is guided by this condition it is guided by this condition ok.

So, this is important findings for electron in a, you will take lattice or electron in a crystal; so, it is energy K the relation is like this. So, that picture has come among from the Kronig Penney model, which is considered for the electron in a lattice electron in a crystal. So now, this picture is it telling that this continuity of this K value it is up to plus pi by 2 minus pi by 2 and then second region plus pi a to plus 2 pi by a and minus pi by a

to minus 2 pi by a this is second region, then third region. So, as you remember that Brillouin zone as we remember that Brillouin zone what was that Brillouin zone. So, that is basically unit cell primitive unit cell in case of reciprocal lattice right, that we cell how it was constructed. So, taking a point and then this nearest points if you add them and then take the perpendicular bisector of those connector and then it will form a boundary enclosed, by this boundary that volume is basically volume or radian for 2 dimensions, it is radian for 3 dimension it will be volume. So, that is basically cell.

So, it is primitive unit cell it will have one lattice point per unit cell. So, similar unit cell in reciprocal lattice same way one can draw, one can find out and that is basically this lowest area or lowest volume in 3 dimensions. So, that is the Brillouin zone and then for next nearest neighbour, if you enclose the volume then that will be the second Brillouin zone of course, just minus this area or volume of the first Brillouin zone. So, that will be second Brillouin zone and there we have seen that if lattice construct for one dimension then the first Brillouin zone is between minus pi by a 2 plus pi by a 2, that we have seen right. So, here you see this K value here whatever we are getting plus pi 8 to minus pi by a. So, this K value this we will tell this is the first Brillouin zone and then this other part this is for second Brillouin zone. So, third Brillouin zone etcetera ok.

So, it is this is called basically. So, it is representing different zones, where this you see this starting of this zone yes discard this flat and end of the zone this are flat, means here gradient is 0 right. Here gradient is 0 rights. So, similarly starting for this second zone with this starting of this is flat and n is flat. So, that is the characteristics of this of this curve E versus K curve and that is important of generation because this will be very useful for our different study. So, this is called basically this curve, contain all the Brillouin zone and it is called the extended zone and now it is possible to bring all these. It is possible to bring it is possible to reduce all these zones, in first Brillouin zone; so this practically so second Brillouin zone is like this third Brillouin zone is like this.

So, as if this second Brillouin zone is taken or reduced in to this first Brillouin zonem third 1 reduced in the first Brillouin zone. So, this is the forth Brillouin zone. So, this picture is called basically reduced zone it is called reduced zone. So, extended zone and reduced zone. So, these all are put in the first Brillouin zone. So, that is reduced zone and whatever this original one so that is called the extended zone. So, now what we want to find out that. So, here you can see this in first Brillouin zone this curve here K is value is

continuous and then here it is discontinuous. So, here this K value is continuous.

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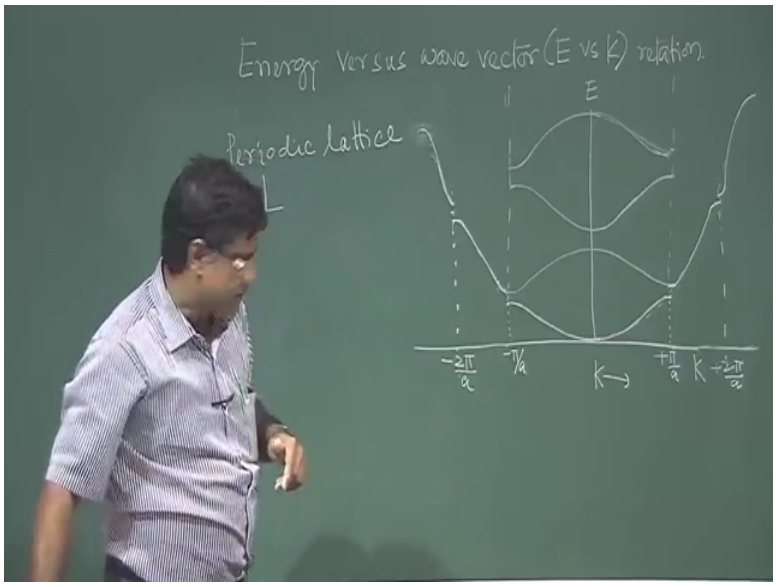

Now you remember that that, we have considered a crystal or periodic lattice of infinite dimension, right; si in a Kronig Penney model considering, the periodic potential of a lattice of a crystal, right. So, there we have considered that the lattice is of infinite dimension. So, there was no restriction there it has the crystal was not of finite size, now question is if crystal is of finite size if we consider the one dimensional lattice if it is length is L right.

Then what will happen, then in this first Brillouin zone. So, how many wave function, how many states how many K value is allowed or we will get in this first Brillouin zone, when our crystal is of finite size say it is crystal length is L ok.

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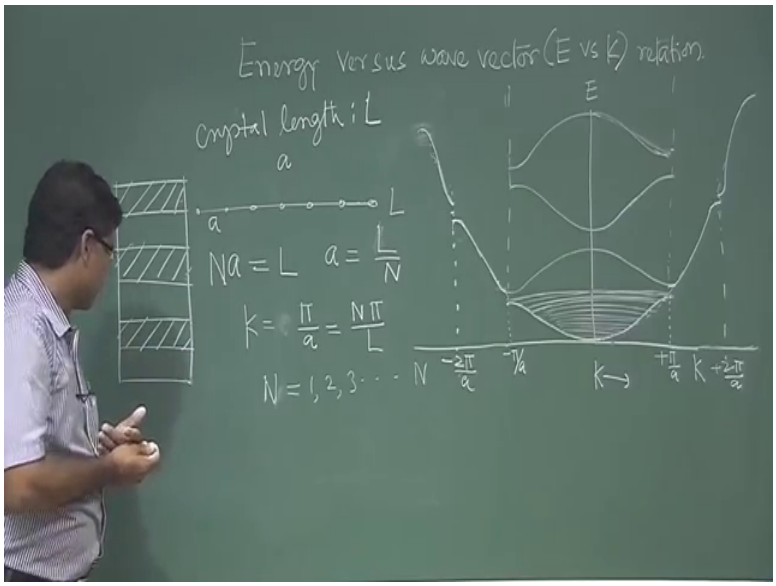

Now, if periodicity of lattice constant if it is a and if n number of unit cell, n number of lattice points are there, n number of lattice points are arranged on this length is L and this lattice distance between 2 lattice points is a and if we consider the primitive unit cell; so one lattice per unit cell. So, what can tell them that how many one can find out, how many unit cells are there in that crystal; whatever we have taken one dimensional crystal length L if lattice constant is a and if we consider the primitive unit cell one lattice point per unit cell. So, we can say that n numbers of lattice points are there, means n number of unit cell we have considered.

So, in that case N a will be equal to this length L right. So, a equal to L by N right. So, here you see this whole K value. So, this in first Brillouin zone this upper limit of K is plus pi by a and minus pi by a. So, when K value is plus pi by a right. So, this you can write or just write pi by a plus minus pi by a or just pi by a. So, then if we put for finite dimension if you put this a value here. So, then what I will get N pi by L right. So, K value is N pi by L right.

So, here what does it mean N pi by L. So, in this region how many n will be how many K values will be there? So, this is the upper limit of K value at this at the boundary of this first Brillouin zone right. So, this is the K value. So, N it can be 2 3 up to N right because when n equal to 1, it is pi by L N equal to 2 pi by L, 3 pi by L. So, I will get many discrete value of K of 2 N pi by L, up to N pi by L that is the highest number right.

So; that means here it is possible to get N number of K value it is possible to get here. So, then you can say that n number of steps, for each value it will represent one state or each K value will represent one energy. So, we will get n number of steps, n number of wave functions in the first Brillouin zone or we will get n number of energy levels right because these, here n number of states are there. So, N number of states so it will have because it is true this for each value of K, it will have different a value right, each K value will give different energy. So, we will get in this region we will get n number of wave functions or n number of steps having different energy and they are not discrete.

So, basically here we get here we will get n number, so it is having low this these zone represents us one band right the second zone represents the second band third band right. So, now here in each band now K values are discrete and it will we will have the energy states. So, many energy states we will get, how many wave function we will, get how many K value we will get, that is equal to the number of the unit cell in our crystal, that will be equal to the number of lattice point in our crystal right and that will be equal to the number of electrons in our crystal. If each in each lattice point one atom are there and that will provide one electron one conduction electron or valence electron whatever.

So, it will contribute one electron to the system. So, thus it is and this is valid for all other or this for second band third band or for second Brillouin zone, third Brillouin zone it will fail. So, each in periodic lattice in a crystal, we are having the band right, now for in finite crystal this band having the continuous energy there is no discreteness, now when we consider the finite size of crystal then it is not continuous, it is it will have the n number of energy levels in this band right, n number of states n number of wave function. So, for each case it will have. So, each band will contain how many number of energy states or wave functions or K value that will be the equivalent to the number of unit cell in that crystal. So, this is very important.

So, this basically from infinite crystal, so you see this form started from free electrons and then we confine them in a constant potential right. Then we consider the periodic potential, but infinite crystal, but then again we are come back to the real system, where crystal have finite dimension, if finite dimension then what happens. So, that is in reality we will have band structure of a crystal and each band will have many numbers of energy states and that number will depend on the how many unit cell present in the or how many lattice point present in the crystal of this finite volume or finite length so.

So, this is the result we got and these here also it is clear that, how the energy is related with this K vector. So, now energy are here each band this energy are discrete K value also discrete.

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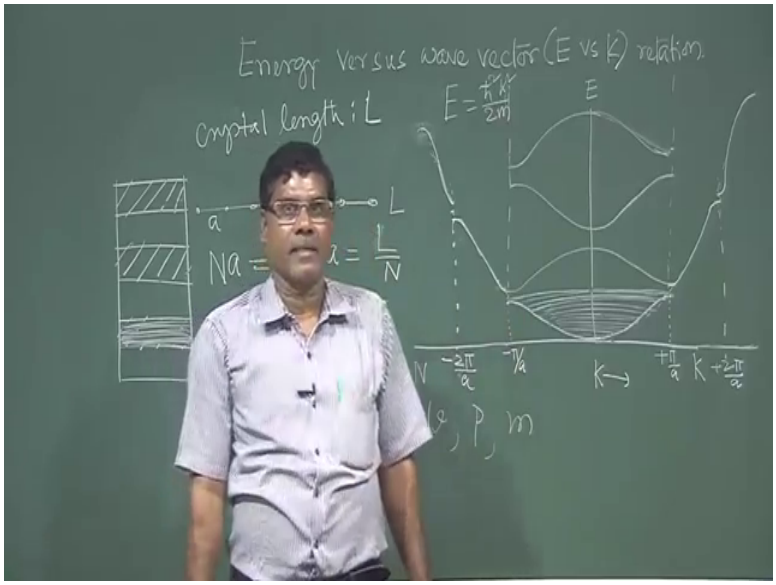

So, this it is defined from the free electron E equal to h cross square K square by 2 m it is different, it is relation is different from them because this relation is gives us continuous variation of energy with K and for real system, crystal of finite length. Now situation is quite different from these pictures. So, this will have effect on the velocity of the electron in a crystal, on the momentum effect of the crystal and then it will have effect on the on the mass of the on the electron.

So, I think I will discuss later on. So, I will stop here.

Thank for your attention.