Solid State Physics
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Lecture - 45
Band Theory of Solids

So, we continue our band theory of solids.

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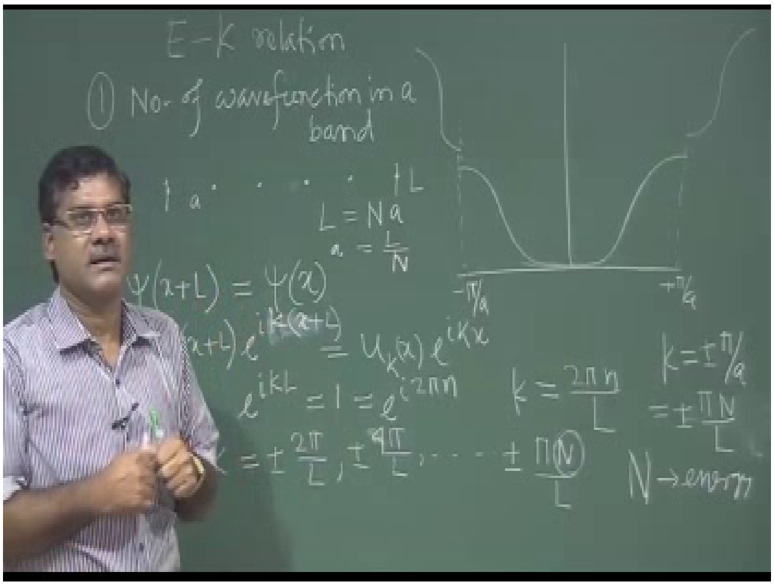

So, you have seen this how band is formed. So, energy versus wave vector relation is very important as I mentioned. So, what we have seen is that there is a break in this E-K curve the curve was, so this kind of this break is there. So, there is a first Brillouin zone, then second Brillouin zone third Brillouin zone. So, each is represent a basically band and this is the band gap, and then another band second band, second Brillouin zone.

Now, in this in this band this first band first Brillouin zone in this band. So, you have energy levels right we have energy levels or so how many energy levels is there is a corresponding wave functions will be there; or case state will be there. So, how many states or wave function or orbitals are present in a in a band. So, that we have calculated in last class.

So, number of wave function in a band if these crystals have a finite length, if the crystal have a finite length. If crystal have a finite length of L, so in this L length there are N number of lattice point, which is separated by distance a periodic lattice one dimensional periodic lattice total length is total length is L total length is L. So, total number of total number of primitive unit cell having a one lattice point that is called primitive in cell.

So, how many cells will be there? So, that will be L equal to. So, each cell length is a. So, N number is cell. So, N a so a is basically L by [noise], and then see if has finite length L. So, it has to satisfy this wave function, whatever wave function number of wave function we want to find out. So, this wave function has to be, has to satisfy the boundary condition psi x plus L, whatever here it is a really take as a ring boundary condition just enclosed it. So, this here whatever value here it has to be same value; so this psi x.

So, the gross function this wave function for periodic potential, this gross function; so this u k x plus L E to the power i k plus x sorry; so E to the power i k x. So, here x plus L equal to u k x E to the power i k x right, so from here you can from this condition you can get i k L has to be 1. So, one means E to the power i 2 phi n, n equal to plus minus 1 plus minus 2 plus minus 3; so E to the power i 2 phi 4 phi 6 phi plus minus. So, it will be one ok.

So, from here this k L equal to 2 phi n. So, we are getting k equal to 2 phi n by L right 2 phi n by L. So, k so for wave function in a periodic potential this it can take k value is plus minus 2 phi by L, plus minus 2 phi by 4 phi by L right. So, what will be it is upper limit? So, it can it can take infinite number of value. In principle it can take infinite number of value, but in these Brillouin zone first Brillouin zone, so how many states are there? So, how many what is the upper limit of this k value? So, in that case this k is; so in Brillouin zone in Brillouin zone k equal to plus minus phi by a. So, that is the boundary. So, that is the maximum value of k ok.

So, this a if we put a equal to L by N a equal to L by n. So, we will get plus minus phi n by L plus minus phi n by L right. So, I we cannot see plus minus phi n by L, this is the maximum number of that is the maximum value. So, in first Brillouin zone that is the maximum number of value; so in first Brillouin zone. So, this k value plus minus 2 phi by L plus minus 4 phi by L (Refer Time: 09:34). So, you can take maximum value phi n by L you can take maximum phi n by L ok.

So, these basically this number this number is so here k it can take maximum how many?

It can take maximum N by 2 right. So, 2 phi n by 2 by L I think that is the so this is plus minus this k value we can take plus minus 2 phi by L plus minus 4 phi by L. So, it is can take. So, these number basically N by 2, 2 phi into N by 2 phi L. So, this these will be N by 2 number total term will be N by 2. So, plus minus are there total N number of k value you will get total N number of k value you will get right.

And corresponding N wave function N number of wave functions you will get, and corresponding you will get energy states or energy it is called orbitals you will get N number of orbitals in a in a first Brillouin zone. Or in a band in any band you will get the number of states number of orbitals, or number of wave functions, that will be equal to the number of primitive unit cell in the crystal of size say L. So now, here so that part I discuss earlier.

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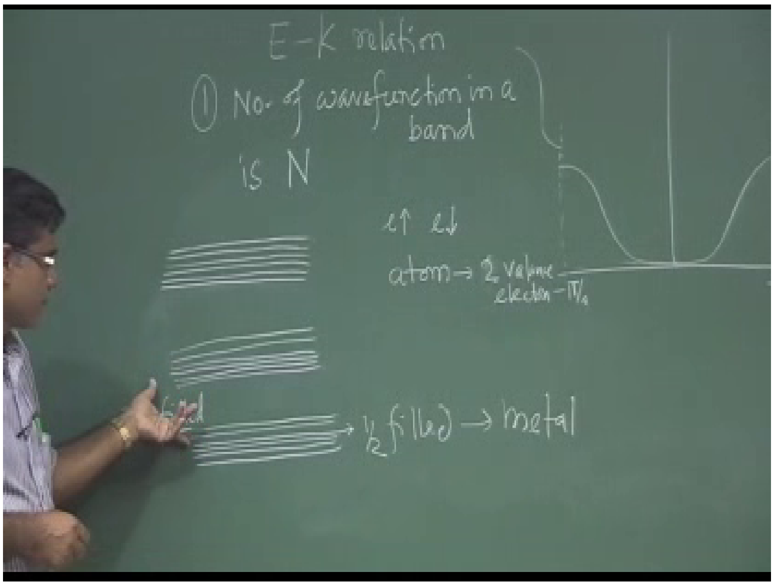

It is important conclusion is important conclusion is. So, number of wave functions in a band is N which is the number of primitive unit cell in the finite crystal. So, you have band right. So, this is one band. So, I think, so we first Brillouin zone second Brillouin zone third Brillouin zone. So, in each Brillouin zone we will get as a energy band. Now how many energy levels will be there? Say if one primitive unit cell in that finite crystal one primitive unit cell.

So, in each band you will get one line, in each band you will get one-line right. So, this for first Brillouin zone second Brillouin zone third Brillouin zone etc there are many bands now if you increase the number of primitive unit cell once by one. So, then for 2 number of primitive cell in each band 2 energy level, if you increase one more. So, you will get 3, you will get 3, you will get 3, right.

So, similarly 4, 5, 6, 4, 5, 6, 4, 5, 6; so that is why these band found. So, number of electrons in each band, how many number of electrons one can one can put so that is electron spin up and spin down. So, in each energy level in each orbitals 2 number of electrons can be put. So, if you take a material if you take a material which is made of a atom which is made of a atom, and that atom has one valance electron one valance electron, one valance electron right.

So, N number of primitive unit cell N number of atoms will be there. So, N number of electron free electron will be there, valance electron free electron will be there. So, this first Brillouin zone they are this first band it will be half filled it will be half filled, because it can take 2 N number of electrons, but our total number of electrons is n. So, it will be half filled it will be half filled ok.

Now, if 2 number so if 2 valance electrons are there, if 2 valance electron are there for atom, then what will happen? Then 2 N number of electrons. So, it will be fulfilled; so half filled, right. Now it is full filled right. Now it is full filled. So, if so other away also if atom is having one valance electron, but atoms basis 2 atoms in one primitive cell it is the lattice one lattice per unit cell, but lattice have a 2 basis 2 atoms. So, then also 2 valance electron per unit cell.

So, you will get 2 N number of so they in that case also it is full filled. Now this wave it is half filled. So, these electrons have. So, all other energy levels are very close. So, it is these electrons can move freely. So, then this type of solid is show the behaviour like metal, when it is full filled, so then that electron it cannot go any higher right to through the only levels are available in the next band, but there is a gap energy gap. So, it has to overcome. So, it is not free.

So, you will not get free electron. So, in that case it is either semiconductor or insulator it is insulator. Now in case of semiconductor at temperature t equal to 0. So, this is waves like it is it is waves like insulator, but at finite temperature say at room temperature. So, it can behave like it will have some free electron, and it will it will behave between insulator and metal; so this so when it is fulfilled. So, it is insulator or semiconductor. So, when it will be insulator when it is band gap this gap is E is quite high. So, then it will be insulator if this band gap is quite small, it is small then it will behave as a as a semiconductor; so in case of semiconductor in case of insulator.

So, this is basically it is fulfilled band. Now to get free electron it has to electron has to move in another band, and that is only possible if band gap is small comparable to the room temperature or slightly higher than the room temperature, then it will it will behave like a semiconductor. So, semiconductor at room temperature at absolute temperature t equal to 0, if it is basically insulator ok.

So, that is what you see this is our when we study this free electron theory, when we study free electron theory, quantum theory, it is quantum theory.

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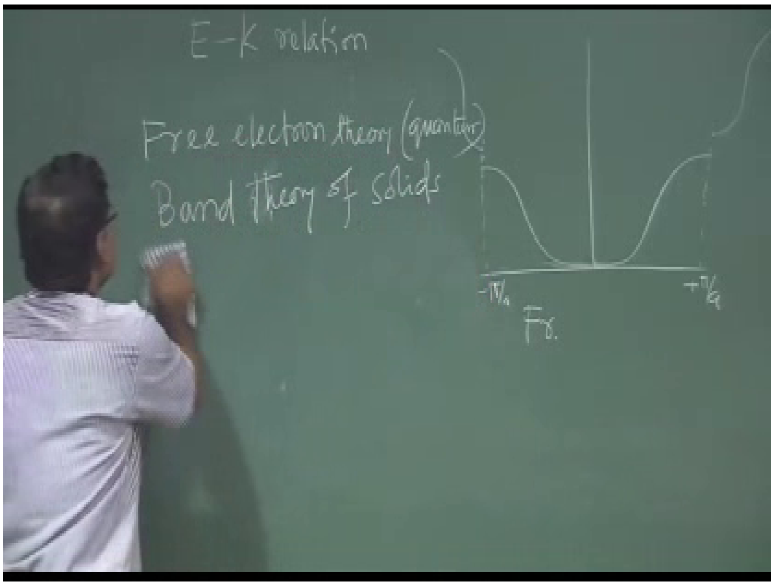

So, then it was able to explain most of the properties of metal right, but it was not able to answer why some material are metal, why some material are insulator, and some materials are semiconductor. So, that answer could not be find from found from could not be found from these free electron theory. So, that is why this band structure band theory of solids band theory of solids are required. And finally, I showed you that this theory can answer why some solids are metals some are insulator and semiconductor, how one can distinguish this solids into in three category based on their electrical conductivity.

So, including this 3 including it can explain this is whatever from free electron theory whatever we go. So, in general this band theory can explain this all materials solids either it is metal or either it is semiconductor or either it is insulator. So, this quite general and successful theory and so in a band what we got in a band, how many number of orbital's are there? States are there? Wave numbers are there? That we got fine.

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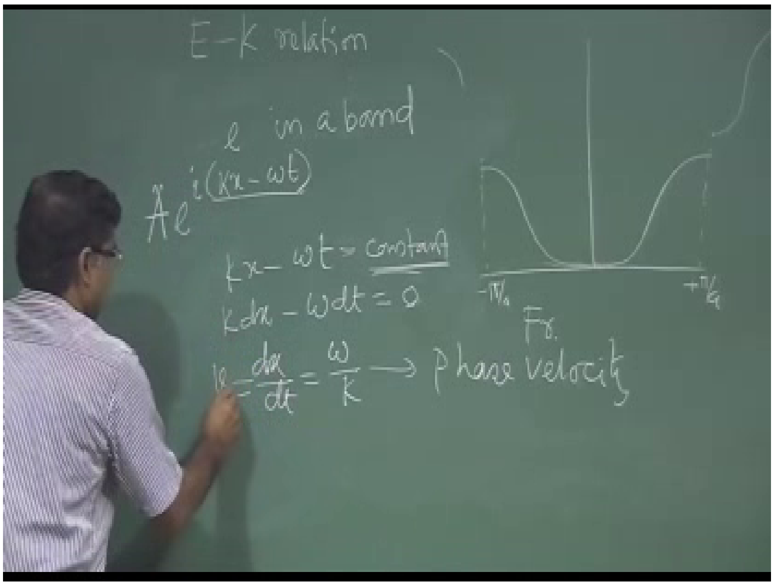

Now when electron can in a band, when a electron in a band, what is your what is it is velocity, whether it is velocity is same as the velocity of free electron or it is different.

So, that we want to find out. So, velocity when electron in a band what is it is velocity. So, basically the plane wave you know travel wave. So, this it is generally we write E to the power i k x minus omega t, that is the wave function for free electron. So, this is basically based faced, this is basically face a x minus omega. It is faced and this is called amplitude right. Now here k d x so if I differentiate.

So, this equal to phase is constant, this is a phase this is a constant. So, when a wave is moving its so we consider that this wave are moving. So, this it is phase are moving, it is phase are moving that phase. So, it is moving such a way it has to move such a way, that is the it is this phase leaving constant. So, we are finding out the velocity of a of wave means velocity of a particular phase, how it is moving with time, how it is moving with time right?

So, we have to consider that particular phase. So, that is why we are considering this the phase is constant. So, differentiate it k d x minus omega d t equal to 0. So, d x by d t is omega by k. So, this is called phase velocity, this is called phase velocity. But. So, this free electron, that free electron which has velocity. So, that is called phase velocity, but when electron in a lattice. So, basically it is not phase velocity, we tell it is a group velocity, we tell it is a group velocity. So, group velocity is defined as group velocity so this is the phase velocity right say d p equal to omega by k, but phase velocity will defined as a b g equal to b omega by d k.

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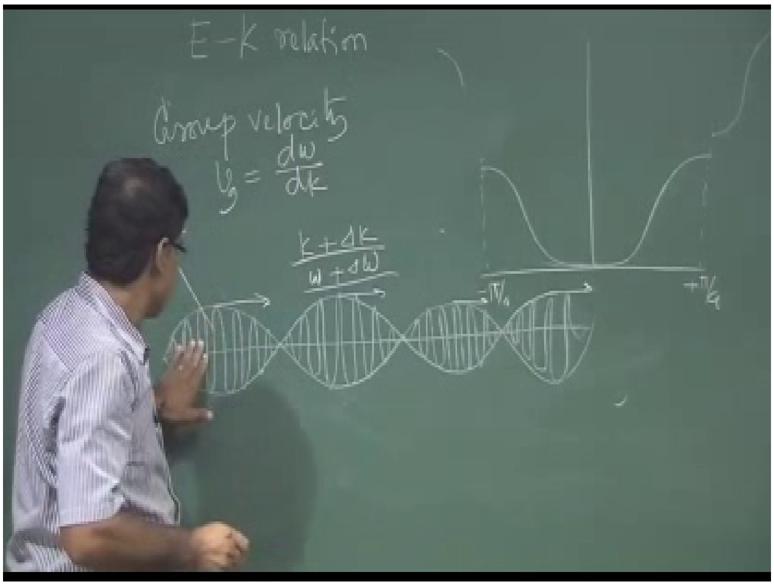

What is that? When this there is a dispersion, when there is not a particular k or omega if there is a so there are many components close to that it is within this. This d omega and d k range. So, it is basically k is not unit k is k plus delta k, and omega is omega plus delta omega. Then you will not simple just plane wave you know, it is not like this it is not like this. So, this wave when there is a dispersion there is a range of omega and k. So, then it is it basically I think so it is going on.

So this type of wave carrier this is like a wave packet and wave packet are moving with velocity with group velocity. So, here you can see 2 periodicity one is this as a whole this is moving. So, this one periodicity is this. So, this is basically phase velocity, these are moving with a velocity that is phase velocity, another as a whole this surface of this one. So, these have also periodicity, these have also periodicity as if this are these are moving these are moving this angle of is moving. So, wave as a whole is moving wave packet is moving wave packet is moving. So, this velocity is called group velocity. So, these basically these that individual this is omega y k this velocity, but this wave are moving with this with this velocity the envelop moving. So, that that is group velocity.

So, in this case wave packet are moving. So, that is a velocity a group velocity, but there also this phase velocity, that that main component that that is that is also a it is moving with the with the packet. So, that is v t with this velocity it is moving. So, that is the good velocity; so when electron in the band. So, it will no longer it is a free electron it no longer it is a free electron. So, it will move with not phase velocity, it will move with velocity. So, b g equal to d omega by d k. So, this g I will remove just v equal to d omega by d k.

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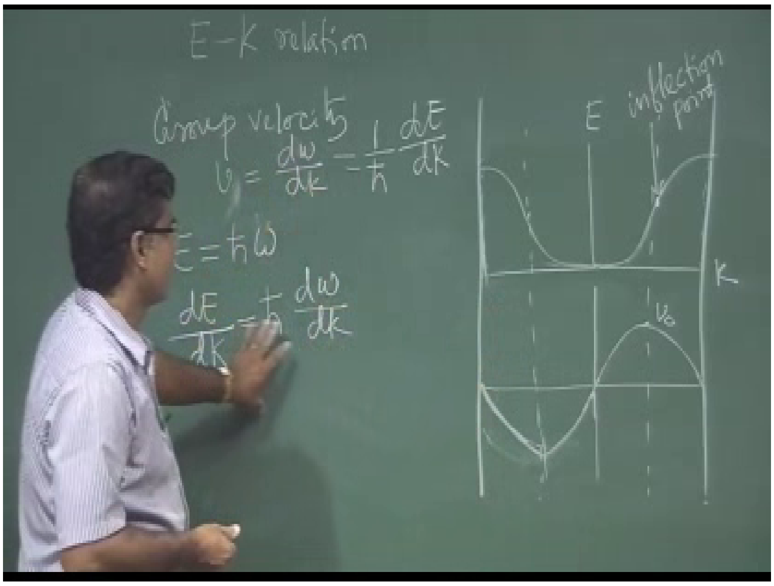

So, what we know about these energy because E-K relation is important as I told. So, this is known to us if known to us E equal to k is cross or h cross k right. So, d k by d E by d k equal to h plus right.

DE by d k equal to h plus. So, sorry so this is the momentum h cross k equal to h cross omega sorry. So, I can so omega is a function of k and E is a function of k. So, I can differentiate d E, E by d k equal to h cross d omega by d k. So, d omega by d k equal to 1 by h plus 1 by h plus d E by d k. So, this is the group velocity. So, if you move the energy a value relation, then you can find out the velocity. So, here justify consider the first Brillouin zone, if I consider the first Brillouin zone. So, here it is first Brillouin zone it is known to us. So, this is the E-K relation right. So, this is E and this is k. So, sorry so here we see this d by d k is nothing but slop of this curve, d E d k is nothing but slop of this curve.

So, here this slope is 0 and then slope is positive slope is positive, then here you see this is one curvature, and then this is another curvature. This is one curvature and this is another curvature this curvature change at this point. So, called this called what is called inflection point, in flection point right. Curvature changes this all inflection point. So, if you if you draw corresponding velocity. If you draw corresponding velocity what will get. So, here velocity 0, because this is 0 and here also flat velocity 0. So, you will get you will get here velocity 0 velocity 0. So, in between you will get maxima and on other side it is opposite it is negative. So, you will get sorry. So, this at inflection point basically this is the inflection point.

So, my drawing is not correct basically, I should draw, I should draw like this I should draw like this, say at inflection point it is it has to be maxima velocity is maximum. So, at inflection point velocity maximum say this is v 0, and others velocity 0 right. This is important relation important findings, now here you see the electron in a crystal in a band now it is velocity it is velocity at the bottom of the band it is 0 or at the top of the band it is 0, but in the middle of the band it is maximum right. So, if you apply electric field. So, then electron will move with some velocity with some acceleration right, but you see it is it is velocity is different in the upper top than the lower bottom.

So, these are the very important findings. So, that is the velocity that is one find out the velocity from this E-K relation.

Thank you. I will continue in next class.