Solid State Physics

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Lecture - 40
Band Theory of Solids

So, we will discuss today Band Theory of Solids.

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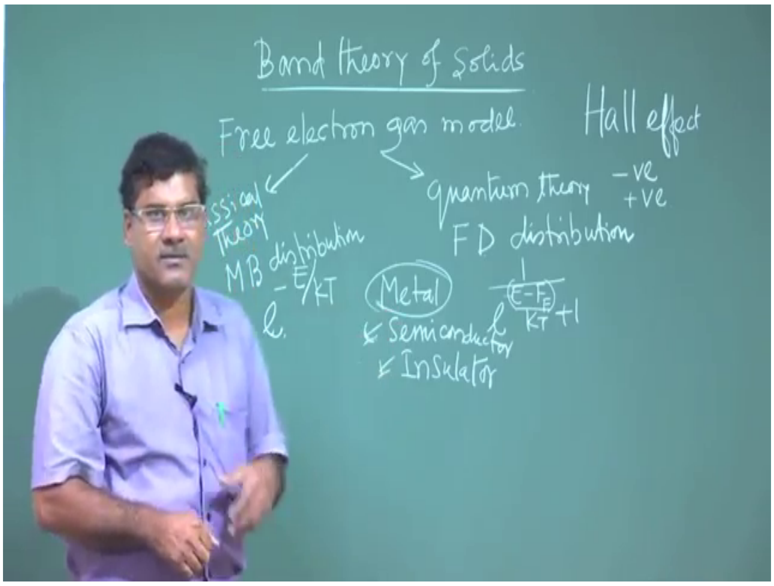

So, for metal we have used free electron theory or free electron gas model and initially, we considered classical theory and then found it cannot explain some all properties. So, then we have considered quantum theory right. So, classical theory they are Max Boltzmann distribution is used how particles or electrons are distributed in different energy levels.

So, they are this Maxwell Boltzmann distribution theory that distribution is that basically, it is this is the factor using this factors or function of energy and, but it is found that it is not correct distribution of electrons because electrons are fermions it is different from the gas atoms. So, appropriate distribution is Fermi deduct distribution. So, that was 1 by E to the power E minus EF by KT plus 1. So, that was the distribution proper distribution and using this distribution we are able to explain most of the properties of metal.

But, now question is then why we need another theory of solids specially to explain this different physical properties of solids including metal and others insulator and semi conductor. So, with respect to that electrical property metal material or solid was divided into three types right metal semi conductor and then insulator. So, most of the properties of metal was explained using free electron theory, but that theory cannot tell that why some metals are very stiff, it is insulating, it shows insulating property or it shows the semi conductor property also probably your you may be familiar with this hall effect if you are not familiar that also fine because I will teach you.

So, considering free electron theory. So, this only negative hall coefficient is we get, but experimental we get both type of hall coefficient positive hall coefficient and negative hall coefficient both type of coefficient we get. So, this theory cannot explain the origin of this another type of hall coefficient. So, only it can explain negative hall coefficient not positive hall coefficient and there are many properties. So, this not the universal or very accurate model which could explain everything specially related to the electrical property thermal property also magnetic property.

So, one thing is clear that in case of semiconductor insulator here definitely this number of free electrons will be very small in compare compared to this metal right in metals this huge number of free electrons are available where as in this 2 cases we hardly find the free electrons. So, it is; so, this theory is it is. So, here; that this theory is not suitable for studying the say electrical property of semiconductor and insulator.

So, we need basically modification of these of these free electron gas model as I mentioned earlier, this gas; this model any model is basically is it based on some assumption based on some postulates and then based all that assumption, we develop the theory and if the theory are can explain the experimental result, then we tell this assumption is correct. But if it cannot explain then this problem with our assumption assumptions are not realistic. So, one has to think and modify the assumption take more realistic assumptions. So, that is the way this model is improved.

So, here also; you have seen this past classical model theory was taken, but it could not explain many things; partly, it was explained. So, then quantum theory, then it is most of the things h was explained. So, that is thus, this model was improved then now there are some things which cannot explain these free electron gas model. So, now, again we have to we have to rethink about our assumption and find out the appropriate assumption or realistic assumption and then we can improve this model. So, that is the next step we are going to do this improve of this free electron gas model and that basically that improved version is called the band theory of solids that is the band theory of solids.

So, if we revisit our assumption of free electron gas model. So, in this case, purely just we have considered the free electron free electron in a crystal.

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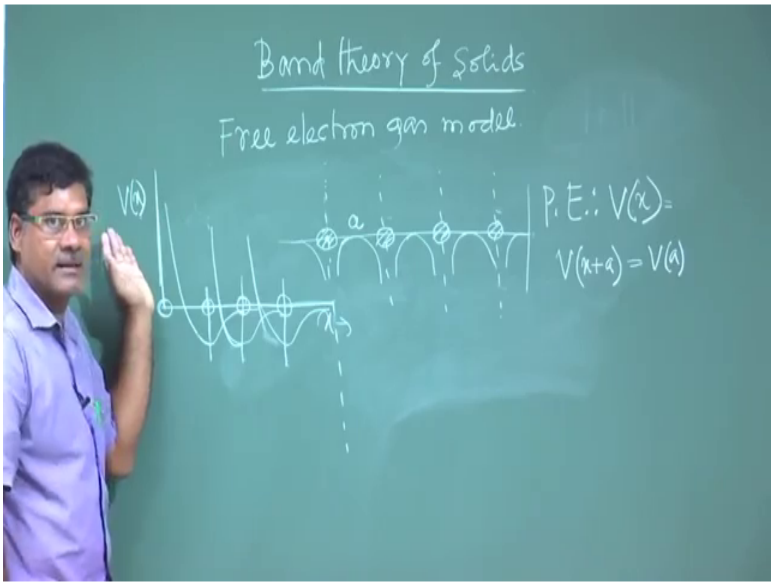

So, we considered it is a; in a box only electrons are there nothing is there no potential energy or constant potential energy one can consider and then based on that assumption we have developed this theory, but one thing we have ignored that it is not a just three dimensional box, it is a crystal, it has latis. So, at each latis points, atoms are there.

So, that free electrons are coming basically from that those atoms, but ions are there right ions are there. So, for each electron there is a ion; there is a ion and they are periodically sitting in the in the crystal they are periodically sitting in the crystal. So, we have ignored the presence of this ions in the in the crystal. And now that was the one that major draw backs it was not the realistic assumption.

So, we have to we have to we have to correct this assumption take more realistic assumption. So, now, in this case if we consider that the error ions the error ions they are periodically arranged in the crystal and electrons free electrons this free electrons when they are moving they are passing through the they are passing through these through this space between among the ions whatever space is available through this it is it is moving right. So, ions have the potential; so, ion that ions in the in the latis points. So, they will they will give potential to the system. Now, which type of potential and how we will consider the potential whether it is constant potential or this potential varies with the distance.

So, that one has to one has to consider. So, definitely there is a potential. So, here we have we have considered we have ignored the potential phase by this electron when it is passing through this ions another also we have ignored that. So, when this; electron are passing through this other electrons are there. So, the interaction with those electrons that also we have ignored. So, in this model band theory of solids in this model now we will consider the potential energy potential energy of the crystal system the crystal system or potential energy in crystal which will which will see this see the electron when that is free electron when it will pass through that system.

So, that potential energy we have to consider and this potential energy if it is a Vx if it is a Vx. So, this Vx equal to whether it is independent of x, then it is constant or it depends it varies with x. So, how it varies that we have to we have to consider and. So, why we should consider the potential and which type of potential we should consider. So, just I can tell you that.

You remember when I have discussed that that when atoms sit in the ordered position in the crystal or one atom another atom being close to that that atom. So, there are some electrostatic force attractive and repulsive force and then we get a balanced position and that is the equilibrium position thus the atom sit in the crystal right it forms the ordered structure of the crystal and in that case we remember. So, when I am bringing this one atom. So, one atom when I am bringing; so, that potential energy it changes, it changes like this that we have seen earlier right.

Similarly, if you bring another atom another atom, so its potential energy with respect to this to its potential energy will vary like this. So, similarly in crystal there are many atoms as it is in a row. So, each one will face potential and this; so, where these atoms are sitting in the crystal; so, where the potential energy is minimum. So, this is say Vx. Now this; I am changing x. So, this potential energy at this site at this site one can get this site are minimum. So, if I consider the lattice; if I consider the lattice. So, joule I can. So, it is lattice row. So, let us take one dimensional lattice, right and then I can consider in that lattice.

So, potential; so, here is I take this 0 level this is 0 level. So, potential i can consider at like this. So, with respect is the negative. So, here potential is lowest. So, potential is lowest. So, here the lowest potential, right. So, here you can see this there is a this basically varying periodically potential is varying periodically this is the minimum potential right then it is moving this maximum potential then it is again minimum then. So, if this the lattice distance a. So, potential is periodically varying here whatever potential after a distance it is coming to the same potential; so if Vx plus a; whatever the potential. So, it will be equal to the Va that is the that condition will be satisfied for these potential in the lattice. So, here we have considered one dimensional lattice. So, there this potential is periodic.

So, I told that in case of free electron gas potential energy was considered constant or 0 that is not correct actually ions are there and their potential varies like this as you have studied earlier and one should consider this potential which periodically varies and it is function of x.

So, that. So, in this model band theory; so, this potential will be considered Vx and that potential is such that it will vary Vx plus a equal to Va right. So, it will; it is periodic potential and so this.

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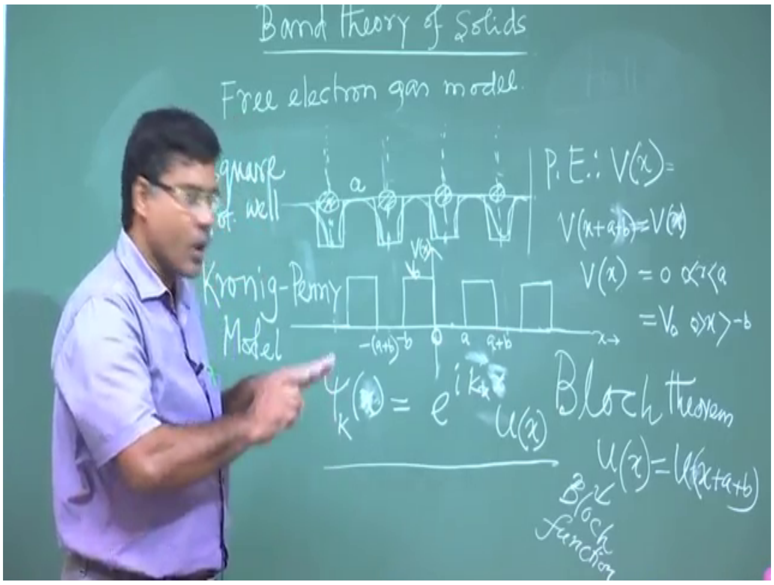

Now, what you what will be the form of this potential what will be the form of that potential that is realistic potential, but problem is mathematically it will be very difficult to handle such potential. So, we have to simplify it we have to simplify it. So, one can consider this potential is say potential is like this, but still it is difficult. So, it has 0 potential for some part and, but this and this say some value V 0, but problem is it is again varying like this. So, it is difficult to handle. So, if we consider this kind of square potential. So, average out. So, it is approximation of this potential to the square potential then we can define this potential we can define this potential this if I take. So, it is V 0, it is V 0 basically minus V 0, it is negative potential, but we if we draw the potential just this way.

So, this level we will take as a 0, if I take this level as a 0, just we are shifting this one this origin so; that means, here 0 potential here 0 potential here 0 potential, then this will be the it was minus V 0 now this will be the V 0 right I can shift the origin I can shift the origin. So, then I can say that. So, now, it is my 0 level now it is my 0 level. So, let us consider. Now, you can see as if this is our ions in at 0 potential at 0 potential ions are at 0 potential.

So, at the ion, it is a 0 potential and then between this 2 ions between this 2 ions be in between. So, there is a potential barrier of height V 0 of height V 0 of I take this is the axis this is Vx; Vx and this value is V 0 this value is V 0 right this value is V 0 and this 0 this is 0 origin i am taking this is 0 this is x varying x fine now you see if I take this, it is a, it is minus b, then this will be a plus b, this will be this is b, this is a minus a plus b. So, these are the ok.

So, a potential is in this case in our case here you see periodicity; periodicity is this, right. So, periodicity is basically periodicity can see a plus b a plus b or this you can see a plus b; so a plus b; a plus b. So, this is that periodicity. So, this Vx; its periodicity will be; oh sorry, here I wrote a, it is not correct, it should be x Vx plus a equal to Vx. So, then in this case in our case the Vx, we have defined. So, periodicity is a plus b V x plus a plus b will be Vx for our system and this V 0.

So, another 2 condition Vx will be 0 when will be 0 when x is when x is greater than 0 x is greater than 0 and less than a greater than 0 and less than a right. So, then Vx is 0 and Vx is V 0; V 0 when x is less than 0 and greater than minus b when x is less than 0 and greater than minus b. So, this is the potential for one dimensional lattice one dimensional solid and under this potential when electron; move through this crystal through this crystal. So, that will be the; that it will face this potential; so this periodic potential.

So, here this square potential we have considered we have assumed this square potential that was assumed by that was square potential well square potential well potential well it was considered by Kronig Penney. So, that is why it is called Kronig Penney model and now for free electron; we have seen this psi k that is we have we have taken this psi Kr psi Kr, you remember we have take e to the power i k dot r right K dot r. So, that was the wave function was taken one as I told; one has to assume wave function proper wave function and then we have to we have to make this wave function for our system considering the boundary condition and other things.

So, first one has to assume a form of wave function looking at the problem within problem. So, for free electron theory we have seen this type of wave function are used this plain wave now here as I told you this that we have free electron that whatever assumption that within is there. Now we are introducing this periodic potential. So, this wave function also it will be close to the; it will be close to this wave function for electron free gas. So, that was wave function for electron free gas.

So, in this case; so, in our one dimensional case; so, one can right ikx; right ikx; so, now, if this was valid for constant potential or the 0 potential. Now you have periodic potential. Now, we have to consider proper wave function. So, now, which type of wave function will be appropriate? So, that Bloch found that for any periodic potential the wave function the wave function this wave function will be modulated with another function will be modulated with another function. So, ux will be modulated with another function ux where ux will follow the; this function will follow the periodicity will follow the periodicity of this of this potential what does it mean.

So, ux will be equal to u x plus a or whatever periodicity in our case this periodicity a plus b. So, a plus b; so, that is called Bloch theorem that is called Bloch theorem that is called Bloch theorem. So, now, things are ready what I need to define the potential that I have defined and we need have to assume a proper we have to choose a proper wave function. So, that also Bloch from Bloch theorem we are getting. So, this we have periodic potential. So, wave function will be of this kind.

So which this ux is the ux is called the Bloch function; this ux is called Bloch function Bloch function. So, I think more or less everything is fine. Now we have formulated the problem properly. Now we have to solve the Schrodinger equation to get the information about the system.

So, I will stop here. I will continue in next class.

Thank you for your kind attention.