Solid State Physics
Prof. Amal Kumar Das
Department of Physics
Indian Institute of Technology, Kharagpur

Lecture - 36
Electrical Properties of Metal (Contd.)

We will continue the free electron model and in quantum theory.

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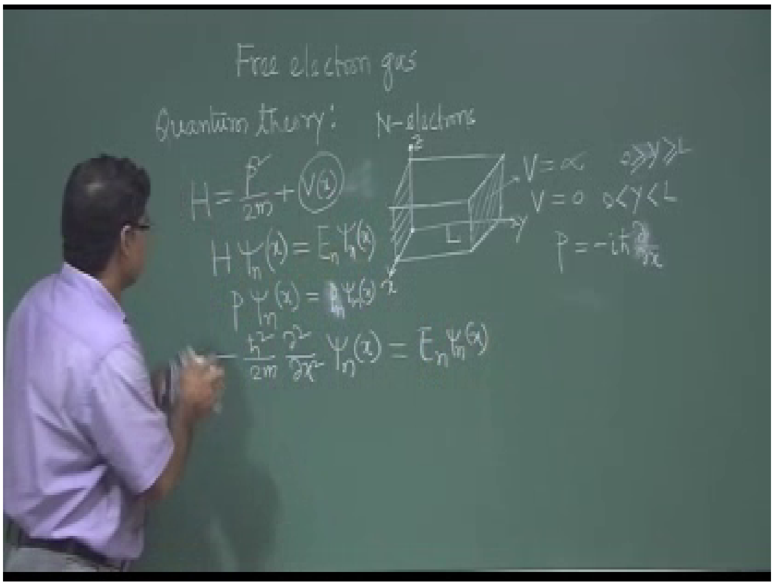

Free electron gas in metal classically we have seen now we have started quantum theory. So, in quantum theory, basically we have considered that the N numbers of electrons free electrons are constrained in a metal box in a metal. So, we can consider that a potential box of dimension L in 3 directions. So, in that metal box what we have assumed.

So, we have metal box. So, we have assumed that the electrons are in 3 dimensional box. It is length if we take this one is origin. So, this direction is x, I think this I can put x this is y and this is z direction. So, length of the box it can be L x L y L z, but for simplicity we can consider cube. So, length in all direction if we consider same L; so these electrons are constrained in this box in this we tell this potential box where electron cannot leave the surface of the metal.

So, along the y direction; so this is the 2 surface electron cannot leave this surface. So, we tell that this just on surface and outside the potential is very high. So, it is infinity. So, in the range of L this x or y whatever you consider here since I have considered y. So, y is less than equal to 0 and greater than equal to L. So, similarly for x direction y direction and z direction one can consider this onto 6 faces the potential is infinity, but since it is free electron inside the box.

So, potential is considered as a 0, v equal to 0. So, inside the box; so this x is greater than 0 and less than L. So, if we consider just one dimension. Later on we can generalize to 3 dimension. So, that in last class, I have shown you that one can construct the Schrodinger equation for this problem. And that really this Schrodinger equation, we write Hamiltonian H it is the total energy of the system. So, p square by 2 m kinetic energy plus potential energy it can be function of x.

So, here y just I wrote, but one can take x also for one dimension. So, that will be the total energy. So, this is the total energy of this system. Now in quantum mechanics you consider the wave function, which will represent the system. So, that psi function is function of x. And it in quantum mechanics it is not only one state it represent it will represent one state, it will represent many states having different momentum different energy etcetera.

So, that is why we put N here. So, N-th state of the system, this wave function, so on this wave function. So, we have to construct the wave function for this system considering proper Hamiltonian for that system. So, generally we tell operator. So, now, on wave function if you apply operator, then this Hamiltonian is basically energy operator if we apply on this wave function. So, if it gives the energy for this state in a state you give energy n. So, this is the basically Schrodinger equation.

So, now H this operator for your case for our case it will be this inside the box this Vx is 0. So, it is just p square by 2 m. Now this momentum operator p, if we apply p on this. So, you will get momentum. You can write p n psi n x right. So, generally we write k, value write k, some h cross will come let us keep it; so these momentum operators. So, it is retained in this form minus i h cross in 3-dimension grad.

So, have been one dimension one can write del by del x. So, if we write in operator form. So, p square by 2 m, it will be minus p is minus i h cross. So, p square i square will give minus 1. So, minus 1 minus plus. No; so p square. So, twice it will come. So, minus plus and now i square will give minus 1. So, it will give minus 1, h cross square h cross square by 2 m is there; so 2 m. So, that will be the and then del by del x. So, del 2 by del x square.

So, that will be the operator Hamiltonian. Now if you apply on the wave function of the system. So, this will give you energy psi n x. So you have chosen proper Hamiltonian for our system here potential energy 0 only kinetic energy are there. So, that we operate on wave function. The form of wave function I do not know. So, that is the task we have to find out form of wave function, for our system. And also form of N energy that I do not know.

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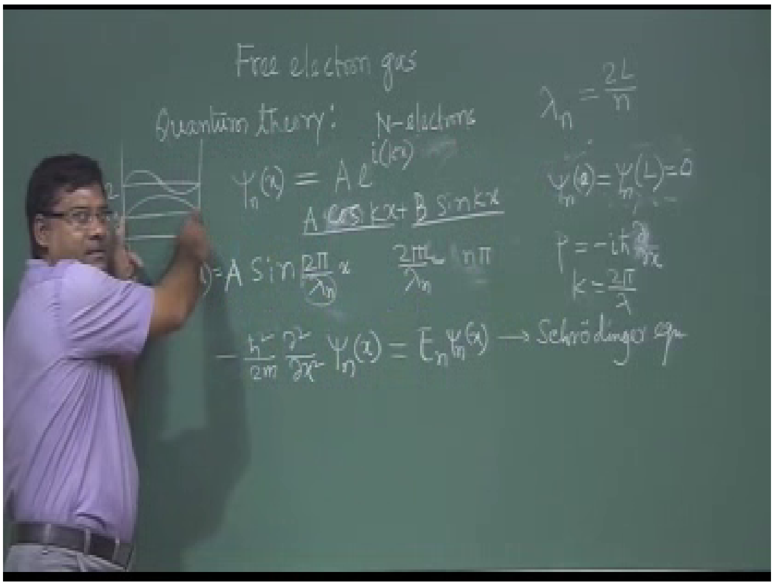

So, that also I have to find out the form of this energy for our system. So, that is the task.

So, one has to solve this Schrodinger equation. So, this is basically Schrodinger equation for our system, Schrodinger equation for our system; now, this basically electrons in a box. So, as I mentioned that electron also nothing but this it is a wave also. So, it is the solution for this kind of equation, this psi x. The solution one can one can just consider. So, generally wave equation only, wave solution you know that is in this for Ae to the power minus e to the power i k x minus omega t right.

So, in our case it is not wave function of time. So, we do not need this part. So, it is N in this form. So, that we write, we can write this e Ae to the power see in terms of sin and cos functions sin k x. I think I have to write cos k x plus i sin k x. So, in general one can consider this a cos k x plus b sin k x. So, this is complex number. So, actually this we take for our convenience, but you have to take basically real part of that for your for your realistic solution.

So, this can be the general solution of this kind of equation. So, one can take more simplified solution also and check whether it works or not. So, let us take a more simplified form of this wave function looking at our problem. So, what is your problem? That wave function psi n x will vanish at psi at x equal to 0. And x equal to L it has to be 0 right. So, that is our system. So, looking at this system at this boundary condition one can guess which type of wave function we can choose, but that may not be final one.

You can choose for simplicity and then you have to find the proper form of the solution. So looking at this if I take the solution is psi n x is in this form sin. So, I will not write k. So, this k general forms. So, I can write 2 pi by k is 2 pi by lambda right. K is 2 pi by lambda. So, it is lambda n. So, for N-th state I writing for N-th state. So, wavelength of this N-th state is lambda n. So, I just replace this k. So, as you know this k equal to 2 pi by lambda.

So, if I take this form. So, you can see that at x equal to 0, this has to be 0. And x equal to L also this has to be 0. So, if I choose lambda in such a way. So, this will be this part will be 2 N pi. So, this part 2 pi by lambda N, if it is 2 N pi, I have to get lambda N, I have to get what is should be the form. So, this should come as a this I have to write I am missing this one x sin 2 pi by lambda N x.

So, when I will put L. So, 2 pi lambda n. So, for L at L it has to vanish right. So, 2 pi L lambda N equal to 2 N pi. If it is the form, then it will satisfy this both condition. You know it will satisfy the both condition. For x equal to 0 it is obvious this will be 0. And for x equal to L. So, if this is 2 N pi, N equal to N is integer. Then it will be for 1 2 3. So, 2 pi 4 pi 6 pi whatever. So, this will be So, then also I am missing actually I can take even N by 2 right.

So, because it will be 0 for pi 2 pi 3 pi 4 pi right. So then I can take in this form N pi, N equal to 1 it will be pi N equal to 2 it will be 2 pi. So, for all this value; so if I take 2 pi 2 N pi, then I am missing this pi 3 pi. So, I have to write N pi. So, then from here what you are getting lambda N, I am getting lambda N. I will write here because I need this value later on; so lambda N equal to 2 L by n; so this for N equal to 1 2 3 4. So, this will tell the wavelength of your state Nm for N-th state the wavelength will be 2 L by n.

So, smallest longest wavelength will be 2 L N equal to 1. So, that will be the longest wavelength, and one can so your system. So, here you can draw right. So, this is a one dimensional. So, N equal to 1 that is the; so 2 L; so 0 to L. So, wavelength of this wave will be like this right. For N equal to 2 sp this for 1 N equal to 1. For N equal to 2, so it will be for N equal to wavelength will be L right. So, one complete oscillation like this right. So, thus 3 4 you can draw you will get wave function having different wavelength. And they vanish at the surface of the metal. In this case of the box surface of the box in this case it is one dimension.

So, what we got? So, our aim is to find out the proper form of wave function for our system and form of energy form of energy n.

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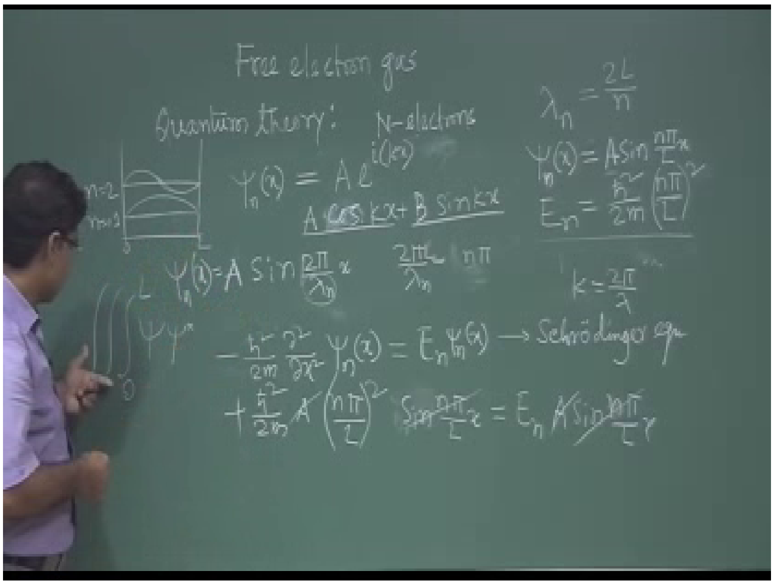

So, here wave function, now I can write psi n x equal to a sin. So, lambda N I will put 2 L by n. So, N will go up. So, 2 n pi by 2 L 2 n pi by 2 L. So, 2 will go and n pi by L. So, I will get A sin n pi by L x right. So, this will be the wave function for our system. So, now, here still that A is unknown to us, other side is known. It is in terms of L dimension of our system is known to us.

Now, A is still is unknown to us. So, that one has to find out for that basically what we have to do for your equation. So, this wave function I have chosen. So, now, that is the form, now it has to satisfy this equation right. This Schrodinger equation it has to satisfy. So, if I put this wave function here. So, minus h cross square by 2 m. So, twice differentiate if you do. So, your A is there and then it will come n pi by L right. Cos n pi by L x. So, n pi by L and again on cos second time differentiation. So, it will be give sin minus sin and then n pi by L.

So, I will get n pi by L square 1 minus sign will come. So, this will be plus this will be plus right psi n x psi n x. So, this in principle I should write sin n pi by L x equal to N A sin n pi by L x right. So, from here what I am getting. So, En. So, you remove this both side. So, En will be equal to En will be equal to h cross square by 2 m, h cross square by 2 m n pi by L whole square right. So, that will be the energy of the [noise]-th state of the system of our system.

So, now it is in terms of all known quantity. We know the mass of the electron; so this length of our dimension of our system that is known to us. So this is the energy of the system. So, one can find out this A. So, that one has to normalized it what is the normalization basically this psi n actually it is repeating the one electron you know. So, I have many electrons. So, here we have considered for state for one electron; so for one electron. So, that will be within the box within the metal. So, the probability to find out the electron within the box, here within this length L has to be 1.

So, that probability is basically psi, psi star whatever the wave function psi psi star. Then one has to integrate what is in our case this is 0 to L within this length it will be there if it is box 3 dimension. So, one has to take 3 dimension in both cases in 3 dimension 0 to L 0 to L or if it is rectangular; so L x L y L z. So, one can consider. So, here it is d x then d y d z if in case of 3 dimension. So, that then one can find easily. So, that I will not find out I do not need this value of A, but one can find out easily should I do it.

So, integrate if we integrate. So, from here you will get A square right. And then you are integrating. So, this it will be cross. So, it will be sin square, no it will be sin square psi psi star sin square, sin square 2 sin square equal to 1 minus cos 2 sin square theta; so 1 minus cos 2 theta. So, cos 2 theta because of periodicity it will be 0. And 1 will be there.

So, 1 means it will be within this limit it will be 1 d x. So, it will be L right. So, it will be L and this part divided by n pi by L right.

So, you will get. So, better let me do it.

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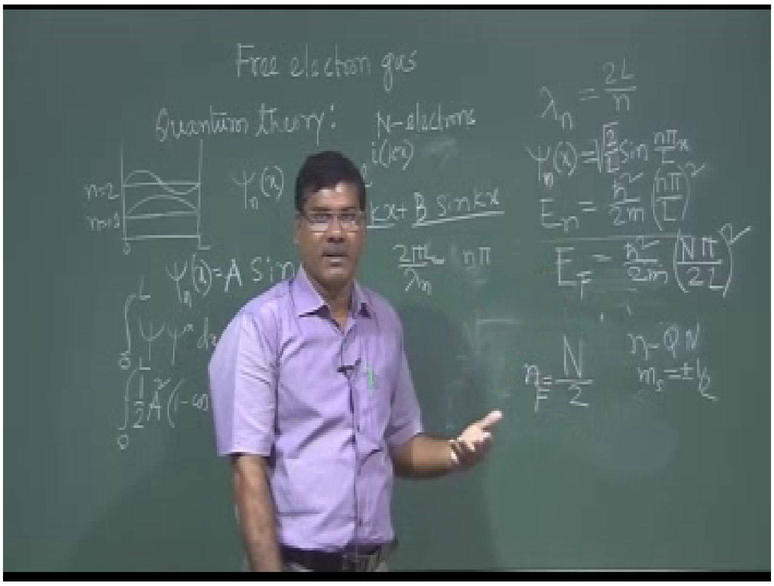

So, this is basically A square, sin square as I told this I will take half. I will take half and then 1 minus cos 2 theta, 2 theta means 2 n cos 2 n pi by L right, x right; so your integration 0 to L; now d x right. So, if you do it. So, what you will get? So, half A square half A square; so it has to be one. Probability to find out the particle within this whole range, within a whole box it will be 1. So, that is the condition of normalization.

So, here. So, if we integrate. So, this cos it will be sin. It will be sin and for 0 limit. So, it will be sin 0 is 0 and for L for L. So, it will be 2 n pi right. So, it is 0. So, this term will not contribute only one d x. So, basically d x 0 to L equal to 1 right. So, you will get this part will give you L after integration, this part will give you L; so here A square you will get 2 by L A square you will get 2 by L right. So, A will be square root of. So, this I one can find out, but I do not need for this problem right now, I do not need.

So, I think we; so our complete. So, put it here 2 by L. So, this is the wave function and energy form of our system. So, electrons in metal if you consider one dimension length are L. So, what is the state of electrons what is the energy what is the momentum etcetera one can find out. If you know the wave function for your system I know a function my system, for my system for one free electron in a potential 0 with barrier infinity infinite potential. So, this is the wave function and energy is this. So, it is representing many states N equal to 1, that is one state N equal to 2 that is another state 3 4 5. So, there are many state.

So, each state we can tell them this is a orbital. It is a energy of orbital where electron can sit electron can stay, but if you have one electron there are many states many orbitals. So, where it will sit? So, when it will sit at N equal to 1 then I will tell it is in ground state; if state stay at N equal to 2 second orbitals. So, it is at higher state it is excited state etcetera. Now if I have N number of electrons, total N number of electrons. So, these electrons I can distribute in this orbitals. Now only this is valid when electrons will not interact with each other. They are free.

So, we have considered for one electron it is free electron. So, we got this one. So, this will be valid for all electrons, if they do not interact with each other as if all are free. So, they will each one will behave the wave we have proceed. So, then for each electron we will get this type of states right. And so we can place any number of electron. So, now, for the system of N electrons, it is a free electrons in a metal in a box or in a in one dimension now how they are distributed.

So, I have now all states or orbitals and we know the energy of the orbitals right. Now I can distribute. So, now, here we have to consider Pauli Exclusion Principle right. All electrons I cannot put in N equal to 1 right. Maximum how many electrons you can put one electron we can put. So, I need N number capital N number of orbitals for N electrons. Now here we consider another fact that that electrons have 2 states spin up and spin down. So, we consider this is nothing but the quantum number.

So, N is quantum number N is principle quantum number. And another quantum number for in our system, we can consider that is m s can be can have 2 value plus minus half. And N can have value positive integer right. So for each orbital for N equal to for one value for each orbital we can put 2 electron one is up and one is down. So, these are valid this Pauli Exclusion Principle is valid for atom for molecule and for solid also.

So, I can put. So, I need N number of orbital as I told, but now I need basically N by 2 numbers of orbitals to put all N number of electrons there. So, what will be the uppermost? So, what will be the uppermost level fill level? So, that will be the uppermost fill level, because I need N by 2 number of orbitals to put N number of electrons there. Because in each orbital 2 electrons are there right. So, I need basically N capital N by 2 number of orbitals. So, that will be the N equal to. So, N equal to N equal to N by 2 that will be the topmost filled electrons.

So, that is the that we tell generally fermi level. That we write in terms of nf, we tell this that is the topmost fill level that is the fermi level above that level is complete lengthy below of that level completely filled up. So, now, you can find out for this nf, what is the energy. So, that is called fermi energy that is called fermi. So, nf. So, n equal to N by 2 think I will write. So, we write this fermi energy that is for n equal to N by 2, I can write h Cross Square by 2 m n equal to N by 2 capital N pi by 2 L square that will be the fermi energy.

So, these are very important term fermi level fermi energy for a solid system. So, really we have we could find out from this simple treatment. So, I will stop here. I will continue in next class.

Thank you for your attention.