Introduction to Quantum Mechanics
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Lecture – 02
Electrons in a metal: Density of states and Fermi energy

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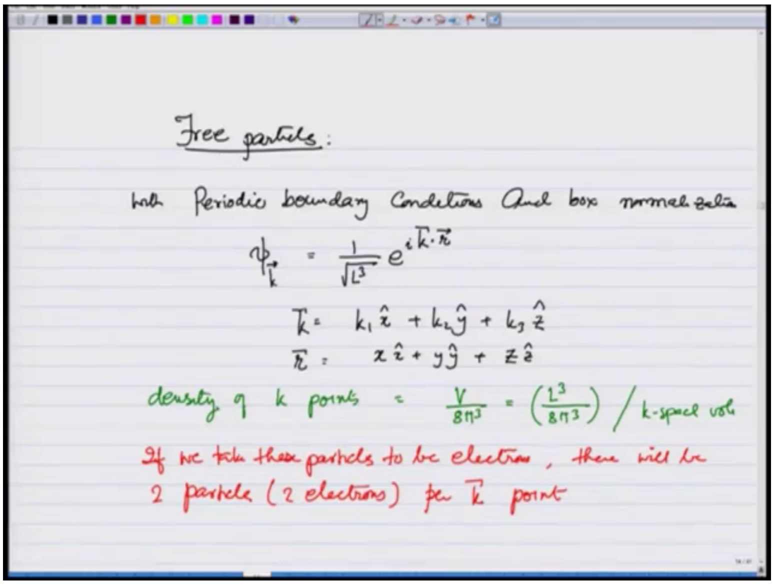

In the previous lecture we learnt about free particles and we said that with periodic boundary conditions and box normalization. We have the wave function psi and I just level them with k, because k itself gives the energy also as equal to 1 over square root of L cubed e raise to i k dot r, where k vector is k 1 in the x direction plus k 2 in the y direction plus k 3 in the z direction, r is x plus y plus z. And the density of k points is v over 8 pi cubed, which is same as L cubed over 8 pi cubed. That is the density of k points in k space this is per unit of k space volume and if we take these particles to be electrons. Then there will be 2 particles or 2 electrons per k point.

Each state can maximum accommodate 2 electrons and therefore, the k space is going to be filled up to somewhere in very large value of k. And this is what we are going to determine in this lecture.

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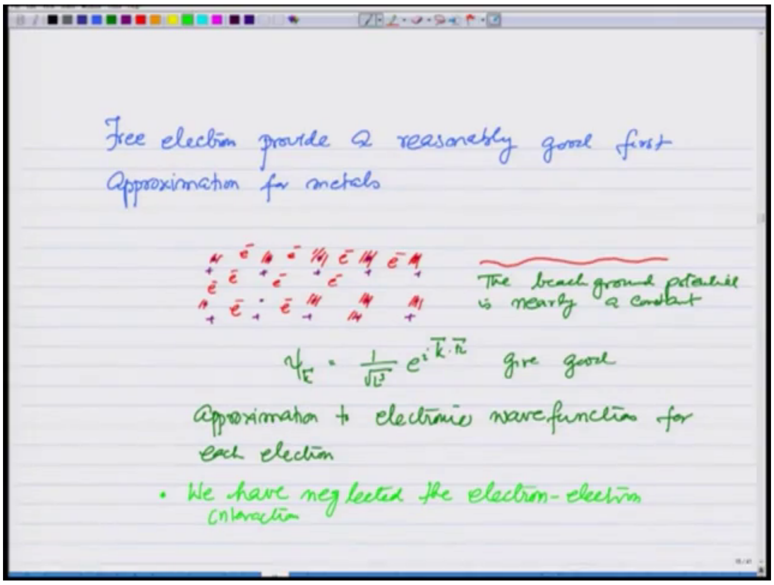

So, this as I said earlier. So, free electrons provide a reasonably good first approximation for metals. Let me argue that why. So, metals are going to have these irons which are positively charged that we make a few and these electrons which are delocalized moving all around.

Since they are mobile what they do is they screen out the charge of the irons. The kind of move around these charges the positive background charges. And therefore, the potential in which they move in a self consistent manner is very much constant. So, potential could be something like this. So, what we can say is that the background potential is nearly a constant for the metals. And therefore, psi k equals 1 over square root of L cubed e raise to i k dot r give a good approximation to electronic wave function for each electron. And this process we have also done one more thing and I must point that we have neglected the electron electron interaction. And it turns out that even this is a reasonably good first of approximation.

So, we are going to focus strictly on each electron having an individual wave function e raise to i k dot r, neglecting the background potential which is nearly a constant metals and neglecting the electron electron interaction.

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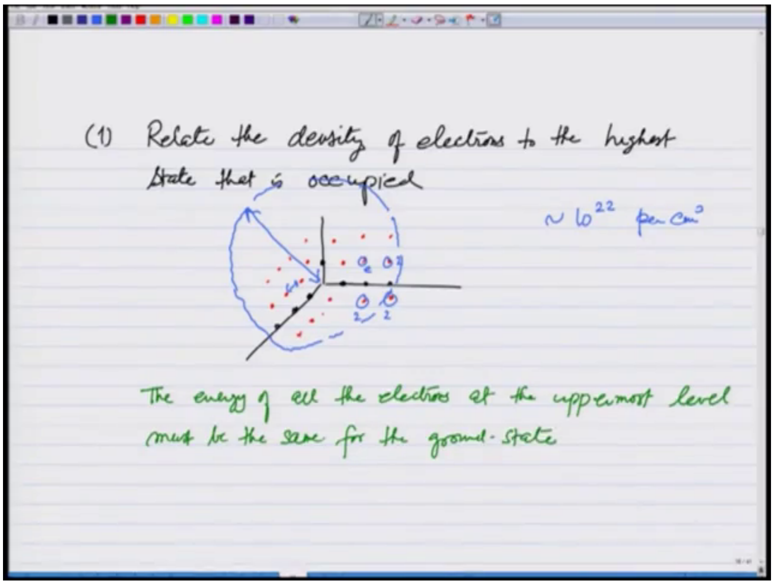

So, very first thing I am going to do is relate the density of electrons to the highest state that is occupied. Let me explain. So, as I said earlier if I look at this case space every 2 pi by L there is one state. So, let us make these states. These are all filled; however, each state can take only 2 electrons. So, this is 2 electrons, 2 electrons, 2 electrons, 2 electrons in a metal bulk there are huge number of electrons of the order of 10 raise to 22 per centimeter cubed. So, I read of the order of 10 raise to 22 states to fill per centimeter cubed I need that money state to fill all these electrons.

So, all these states are going to be filled. So, what I am going have finally is go to a huge n value. And n varies only by one. So, this is going to be roughly filled like this. Little up and down is coming because n changes by 1. And the scale is huge I mean I made this blue sphere to be radius only to shown by this arrow, but consider this I am considering to be 1, difference between 2 points to be 1, this is going to be huge 10 raise to 20 3. So, this is a huge sphere, now why is it is sphere? Because the energy of all the electrons at the upper most level must be the same for the ground state. Ground state by the definition is the lowest energy state, if some electrons are at higher state energy and others are at lower the electrons from higher state energy can dump come down to lower state energy and lower the energy of the system.

Finally until all the uppermost electrons have the same energy.

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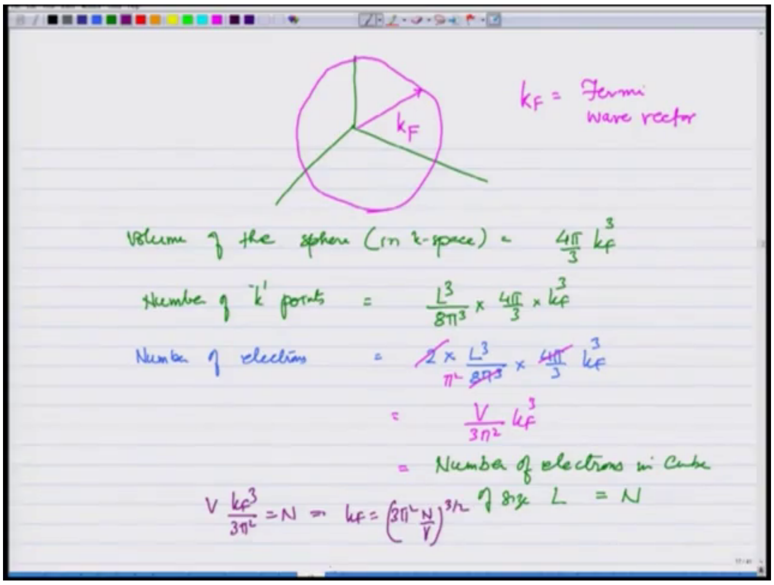

So, what we are going to have is that in this case space electrons are going to be occupied to a good approximation as sphere up to a highest k would also called k Fermi. This is known as Fermi wave factor k, k f is known as Fermi wave vector. So, the volume of this sphere this is in k space is going to be 4 pi by 3 k f cubed.

So, number of k points and this is going to be the density of k points L cubed by 8 pi cubed times 4 pi by 3 times k f cubed. Because we have seen that per unit volume of k space the density of k points is L cubed over 8 pi cubed. And each state carries 2 electrons, so number of electrons is going to be 2 times L cubed over 8 pi cubed times 4 pi by 3 k f cubed.

And if I cancel a few terms 2 and 4 pi goes this becomes pi square I get v over 3 pi square k f cubed. And this is since I have box normalized over L this is equal to a number of electrons in cube of size L which is n right. And so, we had taken these way function we have counted this state's corresponding to the way function which have been box normalized over L and therefore, the number of k points came out to be whatever we have calculated, and that should be the number of electrons n in this.

So, we have v times k f cube over 3 pi square equals n, or k f equals 3 pi square n over v raise to 3 by 2, let me show this pictorially.

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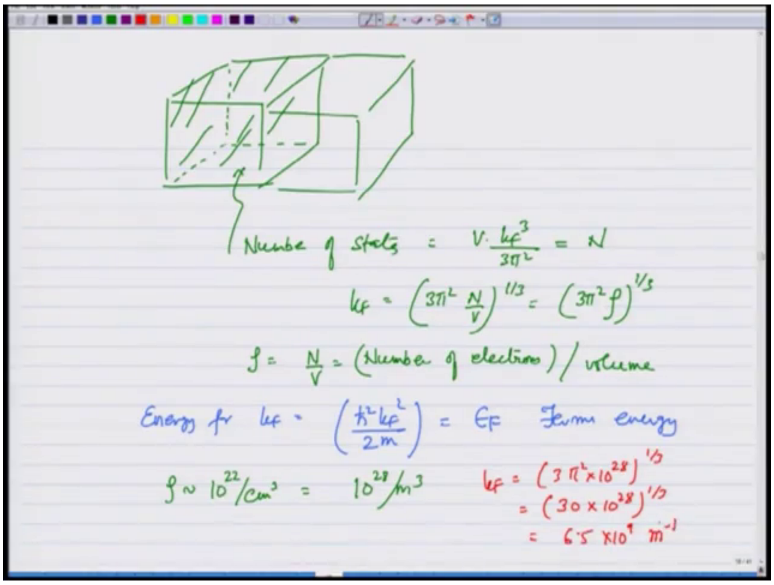

So, I have box normalized over this cube of size L and then it keeps repeating and so on. So, according to normalization over this box. The number of states come out to be v time's k f cube over 3 pi square including the 2 electrons per state and this equals the number of electrons in this.

And therefore, k f comes out to be 3 pi square n over v raise to one third which is nothing but n over v is the density of electrons. So, this is going to be 3 pi square times the density rho raise to one third where rho is n over v is equal to number of electrons per unit volume.

So, we have related what is the highest occupied k vector and the corresponding energy for k f is given as h crosses square k f square over 2 m which is known as the epsilon f of Fermi energy. Now let us estimate the numbers the density is as I said rho is of the order of 10 raise to 22 per centimeter cubed which comes out to be roughly 10 raise to 28 per meter cubed. And therefore, k f is going to be 3 pi square times 10 raise to 28 raise to one third. So, pi square reflect 10. So, I write this as 30 times 10 raise to 28 raise to one third or 300 time 10 raise to 7.

So, that is 10 raise to 9, and for 300 I am going to have about 6 7. So, about let us say 6.5 meter inverse k f is this meter inverse.

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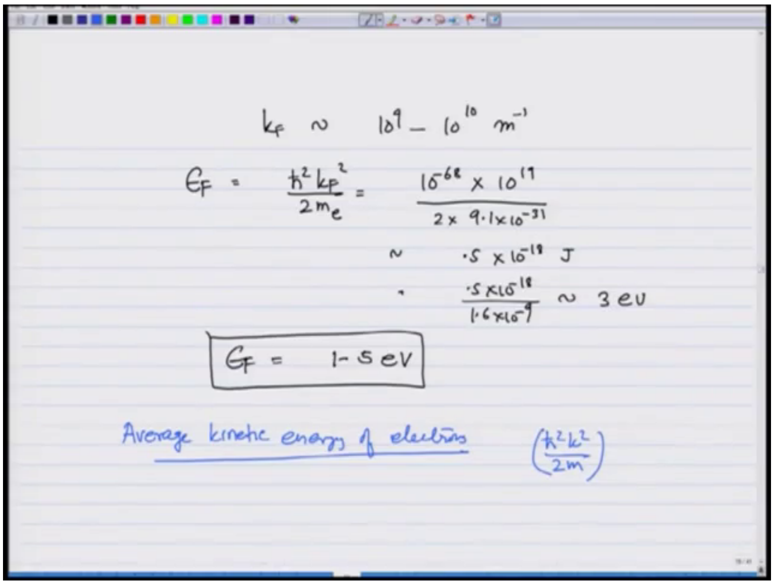

So, we can say that in a metal k f is of the order of let us say 10 raise to 9 to 10 raise to 10 meter inverse and epsilon f is going to be equal to h crosses square k f square over 2 m electrons, which is equal to 10 raise to minus 68 times, let us say 10 days to 18 and 20. So, 10 raise to 19 over 2 times 9.1 times 10 raise to minus 31. Which comes out to be 0.5 times 10 raise to minus 18 jowls which is equal to 0.5 times 10 raise to minus 18 over 1.6 times 10 raise to minus 19 roughly 3 electron volts.

So, epsilon f in metals is of the order of one to 5 electron volts. Given that density another quantity which is of interest is the average kinetic energy of electrons. So, energy of electrons is h crosses square k square over 2 m. And so, it varies from 0 electron volts to 5 electron volts 6 electron volts the highest another Fermi energy and the way you calculate the average Fermi energy is if I again look at that sphere.

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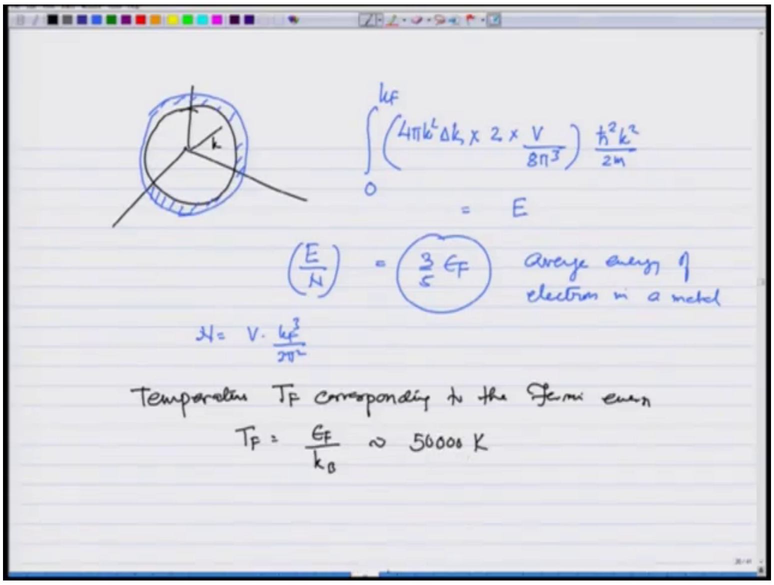

And this sphere of radius k if I take a small shell of thickness delta k, the number of states in this is going to be number of electrons in these state such are going to be such are occupied is going to be 4 pi k square delta k times 2 for this spin times v over 8 pi cubed. And energy of each electron is h crosses square k square over 2 m. And if I integrate delta k being d k from 0 to k f this gives me total energy e of all these electrons. And through this I can calculate E by N which will come out to be 3 fifth of a epsilon f where along the way you will have to write n equals v times k f cubed over 3 pi square.

So, this is the average energy of electrons in a metal. Then if you calculate the temperature T f corresponding to the Fermi energy it will come out to be T f, will be equal to e f over k Boltzmann and you will find that is comes out to the order of 50000 Kelvin. So, what you can see is that if I write the energy on the y axis and fill the states.

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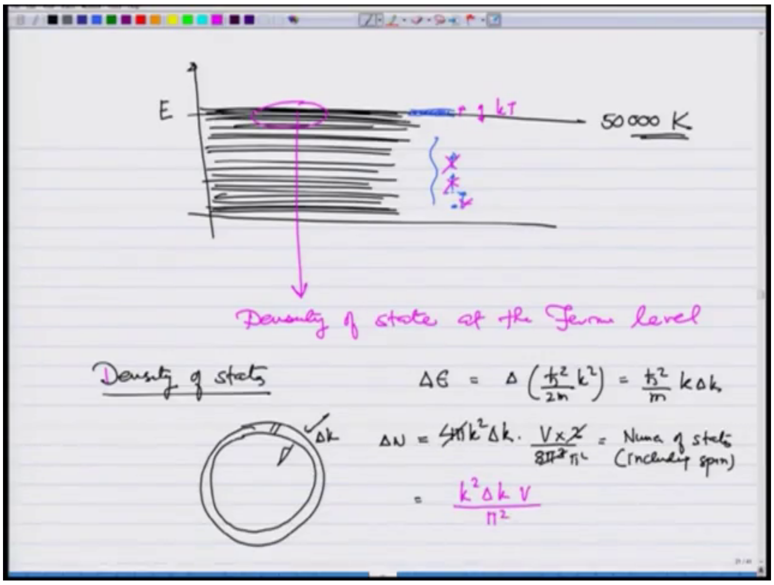

This states that are filled are all the way up to a very high energy value of 1 or 5 electron volts very high energy value because this corresponds roughly 50000 Kelvin.

So, what happens is if I give energy of the order of room temperature, and if I give the energy of room temperature. Electrons that are going to affected are going to be in a very thin shell around that energy. All other electrons are not going to be affected because an electron out here if you take energy k t of the room, temperature cannot go and move to the next level which is occupied. This electron cannot move up cannot move up. So, all these cannot move up, only electron that can gains gain some energies right or top within a thickness of k t.

So, this thickness is going to be k t. So, if I calculate how many electrons are there within per energy range on Fermi level multiplied by k t. That will give me the energy that they absorbed. So, what I need is something called the density of states at the Fermi level. So, that is what we are going to calculate next, the density of states. How do we calculate? Again I will go to the Fermi sphere. And if I take a thin shell of thickness delta k then I have the corresponding delta E the energy equals delta of h crosses square over 2 m, k square which is come out to be h cross square over m k delta k. And the number of states including the spin between these 2 is going to be 4 pi k square delta k times v over 8 pi cubed times 2. This is the number of states including this spin between k and delta k which I can write as delta n.

This cancels for 2, 4 pi cancels at pi square and this I can write as k square delta k v over pi square.

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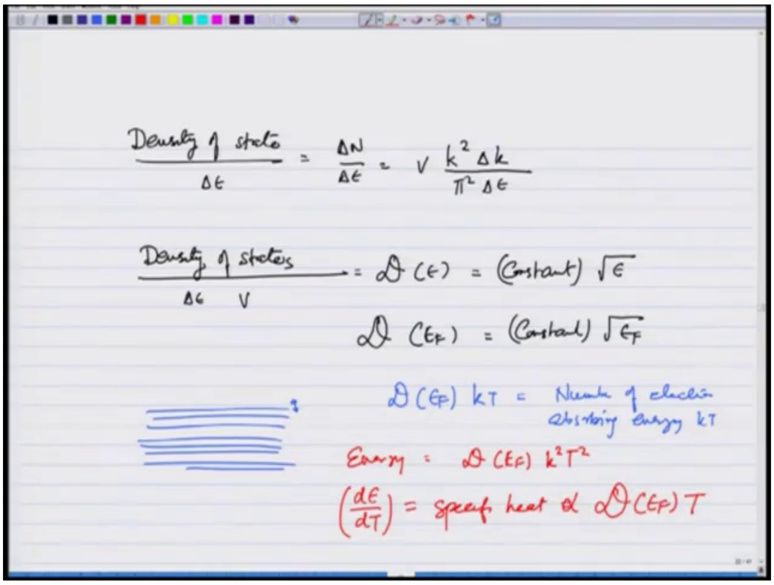

So, if I want to calculate the density of states per unit energy range, delta E will be delta n over delta E which will be k square delta k over pi square delta E times v. So, density of states per unit delta E per unit volume, which is usually written as epsilon comes out to be and I leave it for you proportional to sum constant which depends on m and h and everything times square root of an epsilon. And density of states at Fermi level is going to be therefore, that constant times square root of epsilon f. Going back to that Fermi level being filled now these electrons being filled. And very thin layer out here those electrons getting exited. So, number of electrons exited is going to be density of states at the Fermi level times k t, this is going to be number of electrons absorbing energy k t.

So, the energy itself will be epsilon f d epsilon f times k square t square. And you can see then d E by d t temperature which is specific heat is going to be proportional to density of states at the Fermi level time's t. So, this specific heat of the electrons increases linearly with temperature. And it depends crucially on density of states at the Fermi level, larger the density states of the Fermi level more the specific heat; that means, larger the Fermi energy more the specific heat. This is just to tell you how the filling of electrons how density of states comes into the picture.

Any other transport phenomenon energy phenomena as again going to be confined to very thin layer near the Fermi level, so with this I stop this brief introduction to metals and conclude this lecture by stating that number one, free electron or which is also known as free electron gas provides a reasonably good first approximation to metals.

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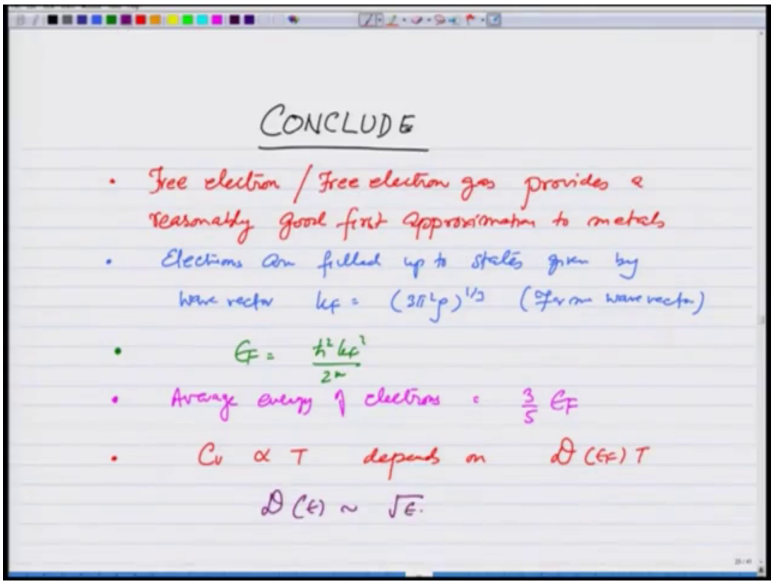

Number 2 is electrons are filled up to states given by wave vector, k f equals 3 pi square rho raise to one third is also known as the Fermi wave vector.

Fermi energy is given as h cross square k f square over 2 m, then average energy of electrons is given as 3 fifths epsilon f. And then specific heat of electron is proportional to t and depends on density of states abs epsilon f, the Fermi level in t and density of states in 3 d was as square root of epsilon.