Properties of Materials (Nature and Properties of Materials: III) Professor Ashish Garg Department of Material Science & Engineering Indian Institute of Technology, Kanpur Lecture 36 -Fermi-Dirac Statistics and Electronic Conductivity of Metals

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So, welcome again to the new lecture of the course, Properties of Materials. Let us just briefly recap what we did in the last lecture. So, in the last lecture, we were talking about, we gave a brief introduction of conductors, semiconductors and insulators. By and large most metals are conductors, semiconductors are known by themselves and insulators are ceramics, ceramics, glasses, plastics by and large. So, and then we looked at the free electron theory of metals. So, here we say that only free electrons or the outermost electrons take part in conduction.

And kinetic energy of electron is given as E is equal to h square, h cross square k square divided by 2 m. And then we saw that if you consider this model and the energy states are also quantised because you if you consider electron as a wave as well as the particle, then electron, let us say electron is sitting in a box and within a box electron cannot be found outside the box of length L, which means it must terminate somewhere here. And since it is a wave, it can have multiple wavelength. So, it can have wavelength like this. So, it can have wavelength like this, so on and so forth.

So, depending upon these considerations, you can have different relations of so, lambda could be equal to 2L, lambda could be equal to L, lambda could be equal to 2 by 3 L and so on and so forth. So, you can relate this to k and we say that k could be equal to, and pi because it is

not only for 0 to L, it could be also for 0 to minus L let us say. So, k can be equal ranging from n pi divided by L to minus n pi divided by L, where n is the quantum number.

So, the energy gets quantised in the form of n square h square divided by 8 m L square. So, the energy quantised energy levels look like this. As you go in space up, so this is n is equal to 1, n is equal to 2, n is equal to 3. So, at the same quantum state you can have 2 electrons, but with opposing spins. So, this is what we did in the last class. Now, so basically, what we are saying is that this is the amplitude and this is x. Now, probability of finding electron is equal to psi psi star or you can say psi square.

Which means if you now, so this is amplitude for let us say and when you square it, after squaring it you will have this relation. Similarly, for if you can square the other one as well, and for the second one your squaring will be like this. And for the third one your squaring will be so on and so for. So, these will be the probabilities. Do not look at the, do not worry about the absolute magnitude, but the probabilities will go like this.

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Now, there is a problem now. The problem is we are saying that probability is equal to psi square, that is square of the amplitude at any point. So, what we are saying is that, for let us say lambda is equal to 2L, probability is maximum at lambda is equal to L. And it is different at different places. So, there is a problem here. This creates a problem because you are having different probabilities at different locations.

So, because conceptually speaking the probability of finding electron must be same everywhere in the solid. Why should you have electron probability maximum in at maximum at the centre but lower elsewhere? So, there is a problem. So, corollary is that we have to, this condition violates, this condition is violated by the result that we get. We get probability, so they are in conflict. There is a conflict.

So, this conflict is, this difficulty is overcome by assuming that electron has, if you consider electron as a wave, you consider electron wave as a, free electron wave as a travelling wave with a constant velocity. So, which means that time averaged probability is same throughout the length of the box or material, you can say. So which means, probability is same from 0 to L. So, this is this conundrum is, this conflict is resolved by assuming electron as a, electron wave as a travelling wave with a constant velocity.

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So, assuming that this is correct, and when we apply this minimum energy principles and in addition to Pauli's exclusion principle, what we are saying is that free electron occupies successive quantum states. So, there are states like, n is equal to 1, 2, 3, 4 and of course you can have distinctions like this.

You can have in one state, you can have 2 electrons that degenerate states. So, basically at 0 k, at 0 k, the highest energy that is highest energy level. So, basically, what is the maximum energy that you can apply, you can occupy? So, at 0 k, the highest energy that can be occupied is called as Fermi energy. So, basically, we are saying that you have this energy states. But at 0 k, there is upper level that is E F. So, E F is the highest state that can be filled or occupied by electrons and this is called as Fermi energy.

So, at 0 k, we say at 0 at 0 k, electrons occupy all the energy levels up to E F. And energy levels above E F so, basically E greater than E F, those states are empty states. So, essentially, for E less than E F, filled states and E greater than E F, at 0 Kelvin. So, this is now when you increase the temperature due to thermal energy, you can excite the electrons from lower energy states to above energy states.

But this basically, what it says that as the temperature is increased, so we are saying that these are the energy states. This is the energy state E F. But you have, you may have energy states above this as well. So these are all filled at 0 k and these are all empty at 0 k. As you increase the temperature, there is a migration of electrons. So as the temperature increases, the electrons go from here to here. So as the temperature is increased, electrons leave lower energy levels and go to upper ones above E F.

So the question is, where do they leave first? Do they leave from here or do they leave from here? So naturally, they will leave from the energy levels which are closest to E F because the energy difference is the minimum. So when you increase the temperature, thermal energy excites the electron which are in the vicinity of Fermi level to the energy levels above it. And this behaviour is, so, which means there is a probability of finding electron above, there is a finite probability of finding electron above energy level, energy levels above E F at a finite temperature.

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This dependence of probability of finding electrons, probability of finding an electron in an energy state at a temperature T is given as f E is equal to 1 over 1 plus exponential of E minus E F divided k T. This is called as Fermi-Dirac statistics.

This is basically probability of finding an electron in an energy, for a given energy state at a temperature. So, this is basically probability of finding electron in an energy state at a temperature T which is f E is equal to 1 over 1 plus exponential E minus E F divided by k T. And E F is a quantity which is, which we take as independent of temperature and it is a material parameter. So, when you plot this, now if you make a plot of now, let us say we make a plot of f E verses E. So, let us say this is the energy E F. If you add 0 Kelvin, at 0 Kelvin you can say, you can write if you, if you write at 0 Kelvin so, this becomes 1 over 1 plus exponential of E minus E F divided by 0.

So, depending up on whether E is less than E F or E is greater than E F, I will have the probabilities appropriately. So, it tells out that f E is equal to 1 for E less than E F and f E is 0 at E greater than E F. So, if you plot now f E verses E, it goes like this. So, this is 0, this is 1. So, at 0 Kelvin, this is at 0 Kelvin, all the energy level below the EF are filled and all the energy levels after E F are empty and the probability at E F is defined as 0.5. That we will see. What happens as you increase the temperature?

So, as at T greater than 0 Kelvin, if you now make a plot of at T greater than 0 Kelvin, the plot, the curve takes a shape which is something like this. So, essentially, this area is equal to, so this is at the temperature T1 which is greater than 0 Kelvin. When you further increase the temperature, let us say this is at a temperature T2 greater than T1. Essentially, what you see is

that, as you have increased the temperature, the probability of finding the electron in energy levels just below E f is lower than 1.

At the same time the probability of finding electron at the energy levels above E f in the vicinity of E f has increased above 0. So, which means all the electrons which have gone to energy levels above E f at finite temperature are those electrons which are in the energy levels residing just below E f. So, essentially, the electrons at any temperature T which is greater than 0 Kelvin, the electrons just below the Fermi energy are thermally exited first and when these energy levels get filled, the electron join the next energy levels in the vicinity of E f and as you keep providing more and more thermal energy, the electrons from the lower energy levels jump to higher energy levels, giving rise to....

But the curve basically, the crossover point always stays at 0.5. So, basically E f is the energy at which f E is equal to 0.5. So, Fermi level is defined as energy level at which probability of occupation of electron at any temperature is 0.5. So, that is the definition of Fermi energy. So, basically, this is what, this Fermi energy thing solves lot of problem for classical physics. Because classical physics that says that all the free electrons can conduct Fermi energy, Fermi-Dirac statistics says that it is not all the free electrons which are able to conduct, it is only those free electrons which are able to conduct, which are in the vicinity of E f.

So, only those electrons which are able to hawk from the energy levels below E f to the energy levels higher E f, they are the ones who takes part in conduction. And this makes lot of sense and this also leads to corrections which earlier models gave in terms of specific heat as well as Hall Effect and this is sort of able to reconcile the experimental observations made in terms of the electronic properties. So, essentially, what we are saying is that at 0 Kelvin, the energy level below Fermi energy are filled and above Fermi energy are empty.

As you increase the temperature, the electrons from the energy states which are just below E f get enough thermal energy to move to the energy levels which are just about the E f. So, not all electrons are moving. It is only those electrons which are in the vicinity of Fermi energy they are moving to high energy levels.

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So, if you look at this in terms of conduction so, in terms of conduction phenomenon what we are saying is that, we saw that K vector can be negative as well as positive depending upon the direction. So, basically if you have electron moving in this direction, the electron can also move in this direction. Okay.

Now, when you apply electric field so, this is what it means you have a, if you have a 0 field, then E k diagram looks like this, which means on both sides we have equal number of electrons. These all are equal areas and you bias the materials when you apply the electric field, electric field what it does is that so, this is your potential energy well. So, when you apply electric field, let us say the electric field vector points in this direction from positive to negative, this is electric field. So, you can see that electron which move from, move to the positive end of the applied field, they acquire extra velocities. So, the velocity of electrons on this side is higher. So, you can say higher velocity, this is E again, this is K and on this side we have lower velocity. You can have other way around as well if you change the vector electric field.

So, basically, what we are saying is that, with this biasing now that we have different velocities of electrons, we are having now motion in one direction, which is because and this leads to conduction.

So, in the unbiased state for every electron moving in this direction, you have another electron moving in this direction. So, basically, kinetic energy is the velocity of electrons are all simpler and as a result, you have no net conduction, but when you apply bias, you have,

basically, you can say, you are saying that you have a equal and opposite velocity distribution in a solid by applying electric field and this gives rise to net velocity in one direction.

So, as a result, you will have net velocity in, essentially, what we are saying is that, net velocity or movement in a direction and this is what gives rise to conduction in a, essentially we are saying that negatively charged, the electrons which are negatively charged particles, they get, they move towards the positive end of the electric field and the velocity of fastest moving electron, electron towards the positive end of E has higher magnitude than the one moving towards other side.

So, this happens in the, this happens only when there are states available above E f. So, basically, if you do not states above E f, if the states above E f are all empty as it happens in insulators, then there is a problem. So, in case of metals, the states are available. As a result, there is no energy gap and hence you can always find states in which electrons can move. So, if you did not have states, this distribution would not have taken place.

So, since you have continuous states, they are quantised but you have states available, electrons can hop. So, as a result, the electrons can move from one side to other and you can have this velocity distribution leading to difference in the, you can have net movement of electrons in one direction.

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So, when you apply electric field, upon electric, upon application of electric field, so we can say that, e E so, this is the electric force. This leads to acceleration of the electrons. So, according to classical mechanics, we can correlate this electric field with the mechanical

force, where m is the mass of electron and a is the acceleration due to applied field and E is the electric field and capital E is the electric field, small e is the charge. Now, what this is saying that, if you keep increasing the value of E, you should get a definite increase in acceleration. So, basically as E increases, a increases but is it true?

They do not, it is found that electrons do not achieve a velocity which is infinite velocity, so reason is no, it is not true because electrons in a solid also undergo collision. So, while electric field increase tends to accelerate them, they do not get indefinitely accelerated because they also undergo collision with various obstacles such as ionic cores, which are positively charged or defects and variety of other things.

So, since electrons undergo collision, so when electron is moving, the electron does not move in this direction. So, you have these atomic cores, so, electrons may undergo this kind of collision. So, these are the collision points which occur. So, as a result, because you can average it out, so we can say that there is average time between two collisions that electron undergoes. So, this average time between two successive collisions is called as relaxation time and as a result, because of this collision because of this balance between acceleration and collision, deceleration caused by collisions, electron achieves a velocity called as drift velocity, which is basically you can say average velocity.

So, this drift velocity is basically the extra velocity that electrons acquire over and above the normal velocity in the absence of electric field.



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So basically, drift velocity is the velocity, average velocity caused by electric field. So, acceleration happen but at the same time, collisions cause deceleration. So we can say that, when you plot this velocity as a function of time, it is sort of undergoes a collision then again decelerates, again and so on and so forth.

So, these are all basically you can say collision. So, there was a starting velocity v, it has reached to another velocity v 1 and the difference is v d. And this time is basically relaxation time. So, in reality, the curve will not be so evenly spaced, it will be unevenly spaced but for the sake of the representation we can say that it is evenly spaced with average relaxation time and average drift velocity.

So, if average time is tau and v d is the drift velocity, then one can write this m into v d divided by tau, which is basically acceleration is equal to e E. So, we can write this v d as, e E tau divided by m. So, basically, electron acquires a drift velocity v d, which is equal to small e that is the electronic charge, capital E which is the electric field, relaxation time tau divided by m which is the mass of electrons.

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So, the current density can be given as, current density can be given as, number of electrons into e into v d. So, number of electrons of charge e moving at a velocity v d. So, this is n e square tau divided by m into E. And this n e square tau divided by m is written as sigma, which is called as conductivity. And this is called as basically J is equal to sigma E. This is called as Ohm's law, geometry independent form of Ohm's law.

So, where sigma is conductivity. This is n e square tau divided by m. So, larger the relaxation time of the material is, larger the conductivity is. More the value of n is, more the conductivity is. So, this tau is a function of temperature, impurity, defects and so on and so forth. So, generally, increasing the temperature, increasing the impurity level, increasing the number of defects leads to more scattering events or more collisions which reduce tau.

So, the conductivity goes down. So, sigma generally of metals decreases as temperature increases, impurity increases and defects increase. So, as you deform the metal, you increase the defect density as a result, the conductivity of a metal goes down. So, so what we have done in this class is, we have looked at the basically the (final) fine contours of quantum mechanics. We basically brought in Fermi-Dirac statistics, which basically tells us the probability of finding electron at various energy levels.

What it does is that basically if you look at just from the electron in a box problem, the electron in a box creates a problem that probability is different at different places, which is not acceptable. So, to overcome that, we treat electrons as travelling waves with constant velocity. So, we say that probability of finding electron is same across the box except at the end it goes to 0, and then we invoked Fermi-Dirac statistics which says that, at 0 Kelvin anything lower than E f is so, Fermi energy is a reference energy which is material dependant.

So, every energy level below Fermi energy is filled but for energy levels above E f are unfilled. And as you increase the temperature, the energy levels which are in the vicinity of E f, they get emptied, electrons from there go to the next Fermi levels, next energy level just above E f. So, only those electrons are taking part in conduction which are in the vicinity of E f. The once which are very low or very high do not take part in the conduction because you do not have any empty states available, you do not have any electrons there.

So, at very high energy levels, you do not have any electrons, at very low energy states, they are all filled. So, only those energy levels which takes part in conduction are those in the vicinity of E f. And then we looked at those electrons which when you have this kind of situation, you create a velocity imbalance. As a result, you have a net velocity in the material that is what leads to conduction of electrons.

And so, when you apply electric field, the electron get accelerated but is it a continuous acceleration leading to indefinite velocities? No. Because when you accelerate electron, electron also undergoes collision with the lattice or defects and this leads to deceleration. So,

as a result, electron basically has a constant velocity called as drift velocity which is electric field dependant.

So, for a given electric field, you have a velocity called as average velocity called as drift velocity. And then based on this, we derive the Ohm's law that is, J is equal to sigma E. we will do more analysis of this in the next lecture. Thank you.