Physics of Materials.
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Model No. 02
Lecture No. 26.
Electronic Contribution to Specific Heat at Constant Volume

Hello, welcome to this twenty sixth class in our physics of materials course. In the last few classes we have looked at the Drude Somerfield model and tried to understand what improvements it has over the Drude model. Specifically, we were able to identify that you know there is density of states expression; that the Drude Somerfield model enables for us to generate. And if you take that into account along with the Fermi Dirac statistics which the Drude Somerfield model creates I mean enforces on system, then we find that the picture of what is the distribution of electrons across energy levels changes quite significantly. So, in this relation we made a couple of different plots.

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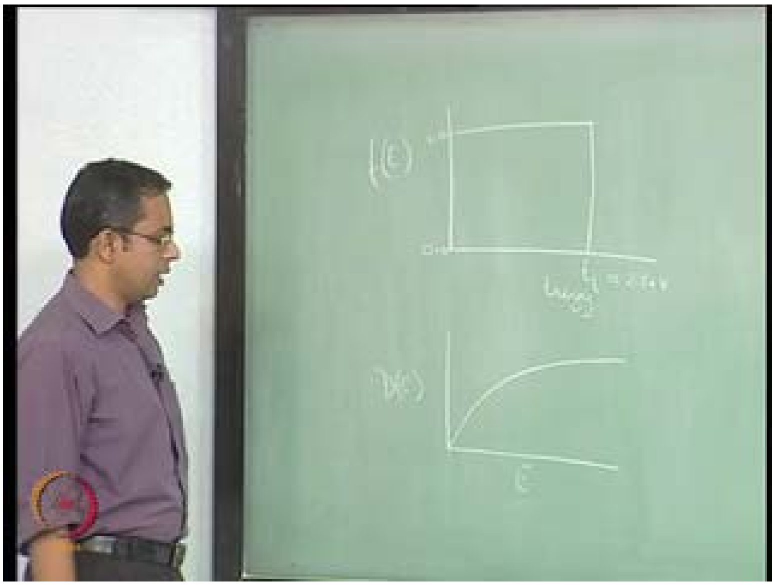

So, we will start with those two plots. We basically said that we have the Fermi Dirac distribution that looks like this. This is energy and this is f of E. So, we have this and this is the E Fermi energy of the order of say 2.5 electron volts. And so, this is the way in which the probability of occupancy is distributed this is the probability of occupancy across various energy levels. And then we also have the density of states which gives us something like this; D of E as a function of E looks like this, it goes as E power half.

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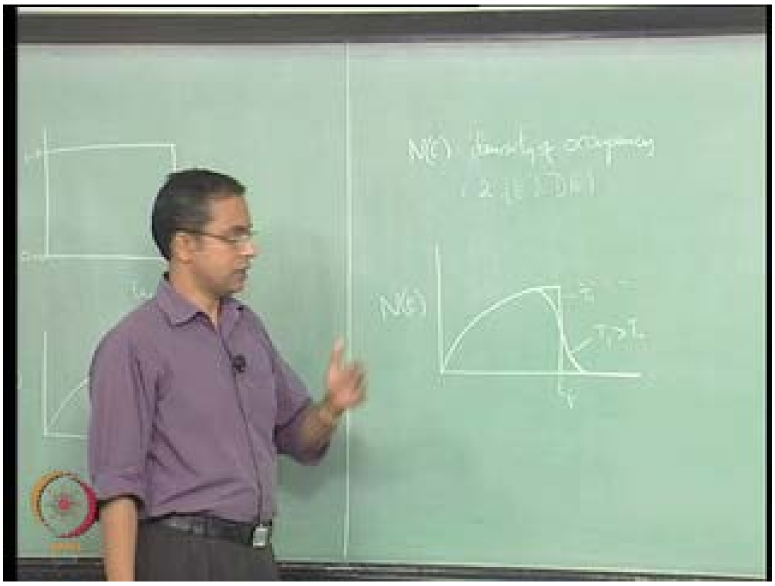

So, you see a distribution that looks like this and then we have the a density of occupancy which is simply two of F of E into D of E, and this two takes into account the fact that we can have two electrons per state if we have not accounted for spin and therefore, you have this function. And so, it is simply the density of occupancy is simply the density of available states times the probability of occupancy. So, we see a behavior that took something like this. So, that is how that would come and at higher temperatures this would just kept modified something that looks like this. So, that is the way it would get modified as you raise the temperature. So, this is at T 0; this is at T 1 greater than T 0.

So, these are the expressions that we have; we use this and a bit often so, we have to just be little cautious on what we are referring to at each state. So that we follow what is going on? So, we will start with the expressions actually for D of E and we also had an expression for the number of available states up to a certain energy level total number of available states.

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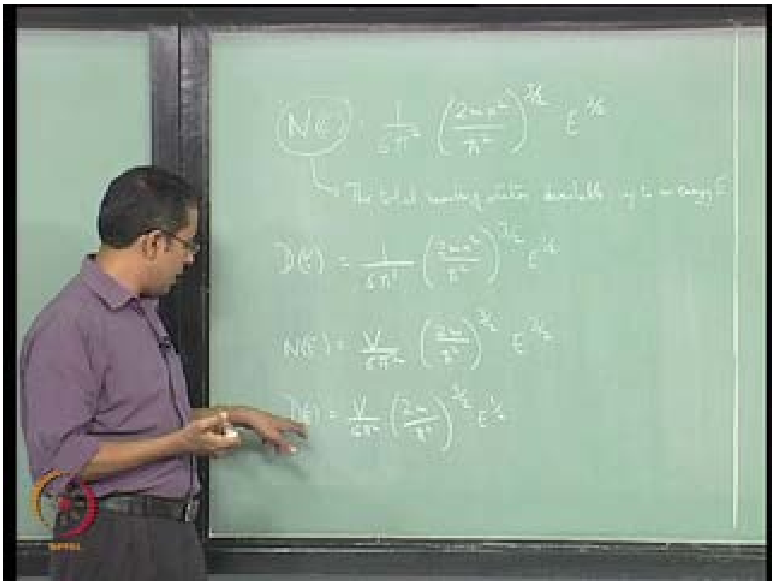

So, those expressions are as we have here we have N of E equals 1 by 6 pi square 2 m a square by h bar square to the power 3 by 2 E to the power 3 by 2. This is now, the number of the total number of states below up to an energy E.

So, this is the total number of states available up to an energy E and we wrote density of states which is simply a differential if you differentiate the expression above with respect to E, we write D of E is simply 1 by 4 pi square. If you differentiate it, 3 by 2 will come here that will become 1 by 4 pi square 2 m a square by h bar square to the power 3 by 2 E power half. So, this is the expressions we have for density of available states and the total number of available states up to an energy E. Incidentally, we can also pull this this a is actually the extent of the system we actually said that the we had looked at the potential well of dimension a and that is how this a came about.

So, if you if you say that that potential well is therefore, the extent of the system. So, to speak this is power a square power 3 by 2 will actually come out as a cube. And that a cube is simply if you want to extend this system into 3 dimensions it is a a cube of volume a and you can think of it as though the particle is now trapped within a cube of volume a. So, that is the manner in which we could look at this. Therefore, the two expression can actually now also be written as N of E is this a square power 3 by 2, it will become a cube which is simply the volume V of the system; V by 6 pi square 2 m by h bar square to the power 3 by 2 E power 3 by 2 and D of E is similarly, V by 4 pi square 2 m by h bar square to the power 3 by 2 E power half like now our.

So, these are the expressions we will use these expressions in a moment for a purpose that we are interested. Our immediate purpose actually is that so far we have descriptively looked at how the Drude Somerfield model actually does a better job of explaining the electronic contribution to specific heat relative to the Drude model. So far, it has as I mentioned it has been a descriptive manner in which we have looked at how it is an improvement. Right now, given that we have these expressions, we can go a step forward and actually try and see if you can put a numerically value down as to how this is actually a better way of looking at the problem that we have tried to address; which is the electronic contribution to the specific heat. So, what we will do is we will now look at this is the density of states at a given energy level E.

So, what is that energy level? We have not specified; it is a variable we have in our system a variable. So, this is the density of states available at that energy level E. Therefore, you can write this in terms of the Fermi energy. So, as we mentioned since the system is built up in such a way that you have energy levels from the lowest energy level available which gets filled up to higher energy level levels and then you eventually you run out of electrons in the system then at that point you reach the highest energy level ava ailable in that system. That highest energy level at 0 Kelvin is the Fermi energy level. Now, given that all those states are occupied when you try to rise the temperature of that system, electrons in energy levels which are relatively low cannot participate in the process.

Because when they gain energy, they will have to an energy level above them, but all the energy levels immediately above them are fully occupied because the probability of occupancy is one. Therefore, only electrons which are very close to the Fermi energy can participate in this energy raise process which is which is occurring as the trial raise this temperature of the system. Therefore, it is of interest to us to first figure out what is the density of states in this case it will it will this is an expression for density of available states but, we are looking at the states just below the Fermi energy and at 0 Kelvin there are fully occupied.

So, therefore, this would also then be the density of occupied states. So, density of occupied states which is very close to the Fermi energy level.

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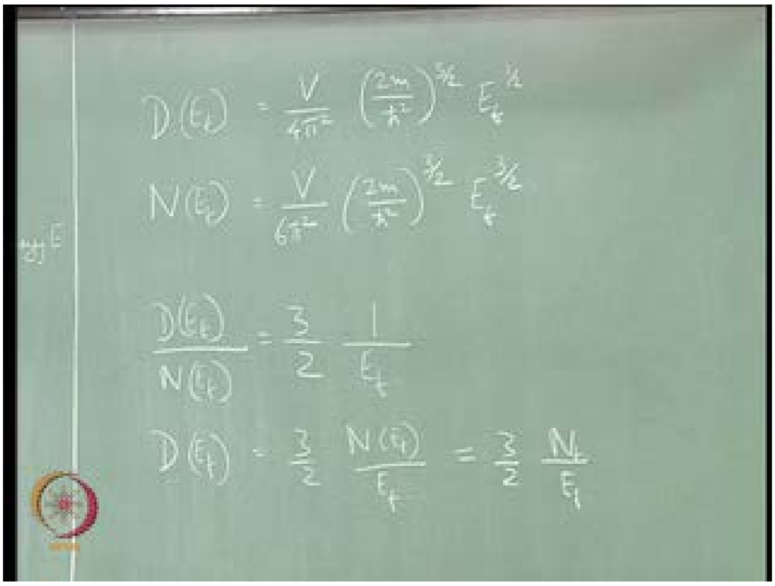

$$D(E_f) = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E_f^{1/2}$$

$$N(E_f) = \frac{V}{6\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E_f^{3/2}$$

$$\frac{D(E_f)}{N(E_f)} = \frac{3}{2}\frac{1}{E_f}$$

$$D(E_f) = \frac{3}{2}\frac{N(E_f)}{E_f} = \frac{3}{2}\frac{N_f}{E_f}$$

So, that is what we are looking at. So, we will write this D subscript E f and so that is the energy level that we are interested in and that is simply V by 4 pi square 2 m by h bar square to the power 3 by 2 and this is E f, the Fermi energy power half. So, this is the density of available states very close to the Fermi energy. And therefore, in fact if we are talking of just below the Fermi energy then, these are also the density of occupied states very close to Fermi energy.

We can also look at the expression for the total number of states that again was written with respect to a general energy that we have not specified; we will now write it as the total number of states available up to the Fermi energy. This is the total number of states available up to the Fermi energy. So, this is what we have; so we have an expression for total number of states available up to the Fermi energy and density of states at the Fermi energy right. So, these are the two expressions we have. What we will do; we are just trying to come up with an expression that is convenient for us in in our final analysis of what is going to happen as you raise the temperature of the system?

So, given the expressions that we have that we are simply going to play with these expressions till we are able to reach something that is convenient for us to interpret or convenient for us to demonstrate what is happening as you raise the temperature of the system and therefore, convenient for us to interpret. So, we will just take a ratio of these many of these terms will therefore, get cancelled so if you write D of E of f divided by N of E of f so you have 1 by 4 here and you have 1 by 6 here. So, it will become 6 by 4 that are 3 by 2. These two terms will simply get cancelled and you have an E power half by E f I mean E f power half by E f power 3 by 2 so that simply 1 by E f.

So, almost all I mean basically most of the terms get cancelled, you just get this constant 3 by 2 1 by E f. Therefore, density of states very close to the Fermi energy is simply the number of states up to the Fermi energy by E f. And these are all calculations we have done I mean so if you think of it as per unit volume basis then this would then be the total number of free electrons per unit volume. Because this is then the density of occupied states; this is now a total number of available states below the free Fermi energy. And since they are all occupied at 0 Kelvin, this this also essentially takes into account, the total number of electrons per unit volume in that system.

So we can also, write this as at least we would be in the right order of magnitude if we write it as number of electrons per unit volume by E f. So, this is what we have. Now, this is an expression we have which we will use; we will go back to our diagram.

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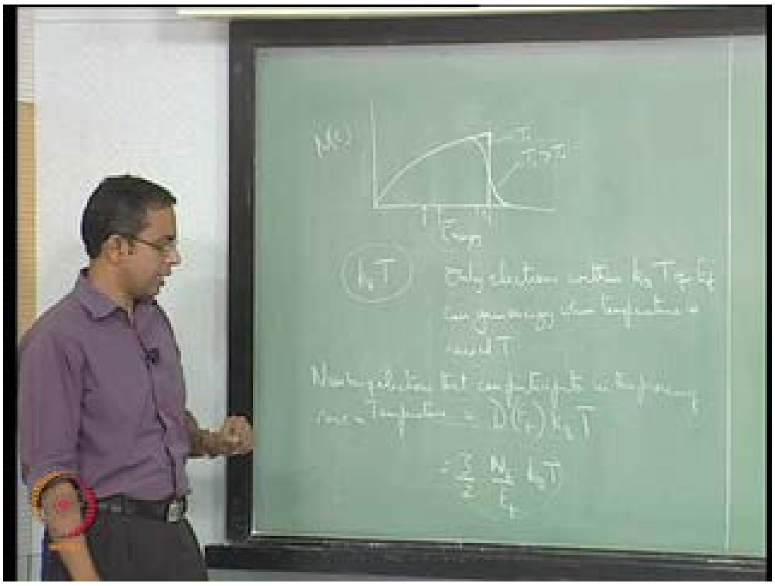

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So, the point we note this is energy of course, is that as we mentioned all the states are occupied up to the Fermi energy level. So, only states very close to the Fermi energy level are in a position to participate the energy raise that occurs in the system as you try to raise the temperature. Now, when you are sitting at 0 Kelvin this is all fully occupied.

When you raise the temperature to T, effectively in terms of a pair electron basis. So, the amount of energy you are providing is k b T of the order of k b T. So, on a pair electron basis of the order of k b T is the amount of energy you are providing in to the system. Therefore, if you see only electrons since that is all the energy you are providing on a pair electron basis, only electrons within k b T of this Fermi energy level can participate in this energy raise system. Because only those electrons can gain this amount of energy and reach states which are empty ahead of them.

If you go further down, there are electrons which in in theory you could add k b T to an electron that is sitting here and that would probably bring it to some position here. Just for illustrative purposes, we will say it is it is an electron that is sitting here and that it is now brought to an energy level that is sitting here. Now, these states are already occupied whatever states are available at that energy is already occupied. Therefore, this electron here is not in a position to gain that energy. In theory, I mean nothing prevents it from gaining the energy, but there is no state where it can go to; it is not gaining energy independent of all constraints; it is gaining energy within the constraints placed on the system. And the constraints ensure that what is ahead of it is already occupied.

So, an electron here cannot gain k b T whereas, an electron which is just within this band within k b T of this Fermi energy can gain k b T and find locations ahead of it which are empty. Therefore, only electrons in our diagram here it is T 1 but, we will say raise to a temperature T; only electrons within k b T of the Fermi energy can gain energy when the temperature is raised to T. So, how many of these electrons are there? To get an idea of that, we simply have to look at the density of the states which is at the Fermi energy level and multiplied by k b T. If you assume that, we are making an approximation here that this drop of is not very severe. See eventually, it is going to drop this way; the number of energy levels is going to drop this way.

So, therefore, the density of density of occupied states density of available states but, it is probability of occupancy is one. So, density of occupied states is going to decrease but, we are saying that the k b T is relatively small number. And therefore, within k b T of the Fermi energy within this k b T of Fermi energy there is not a very significant drop in the density of states. So, the total number of electrons that can participate in this process is the density of electrons available per unit energy, at the Fermi energy times this k b T. Therefore, number of electrons D of E f time this k b T which we have already found is simply 3 by 2 N f by E f time this k b t.

So, this is now the number of electrons in the system per unit volume basis; if you want to say which can now gain energy as a result of the raise in temperature. So, we have a k b T term already here, but this is still this total term that here come works out to essentially is talking of the number of electrons that can participate; number of electrons per unit volume which can participate in this gain of energy as you raise the temperature to a temperature T. So, k b T is the range of energy values over which the electrons can gain energy. Now, we have already seen that the energy of an electron at a temperature T as given by the ideal gas behavior and so on is simply 3 by 2 k b T.

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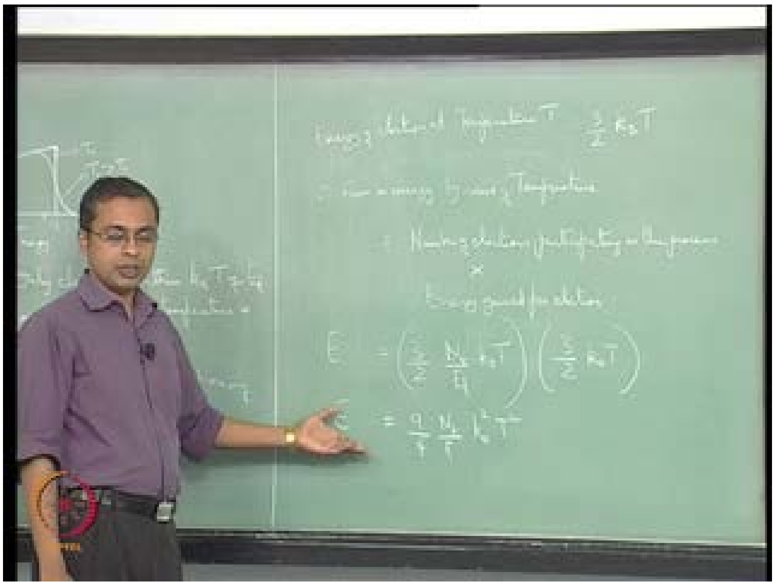

This is the energy associated with an electron; actually energy associated with a particle at temperature T as given by the classical behavior. But we are just assuming that you know the only thing we have changed is the introduction of Fermi Dirac statistics. And therefore, and the quantization but, in principal we will assume that this is still the energy that is associated with an electron at temperature T. Therefore, the gain in energy by raise of temperature is equal to number of electrons participating in the process times the energy gain per electron.

So, the gain in energy due to a raise of temperature for the system is simply the number of electrons participating in this process of this change in temperature, times the energy gained per electron. So, we have now got expressions for both. So, this is simply equal to; so if you want to write this this is E; so this is the energy E; this is the number of electrons participating in the process that is 3 by 2 N f by E f times k b T. That is the first term here, number of electrons participating in the process times the energy gained per electron which is this 3 by 2 k b T. So, this is what we have now got for the expression.

So, we have actually played around with a lot of numbers and expressions, and come up with something that is beginning to look like an expression that we can handle for our immediate purposes. So, if you simplify this expression you have 9 by 4 N f by E f k b square T square. So, this is what we have as the total energy that is being introduced into the system; as you raise the temperature of the system to a temperature T. So, this is what we have got therefore, if you now want to look at the specific heat contribution as a result of this raise in energy; we simply have to differentiate this with respect to temperature.

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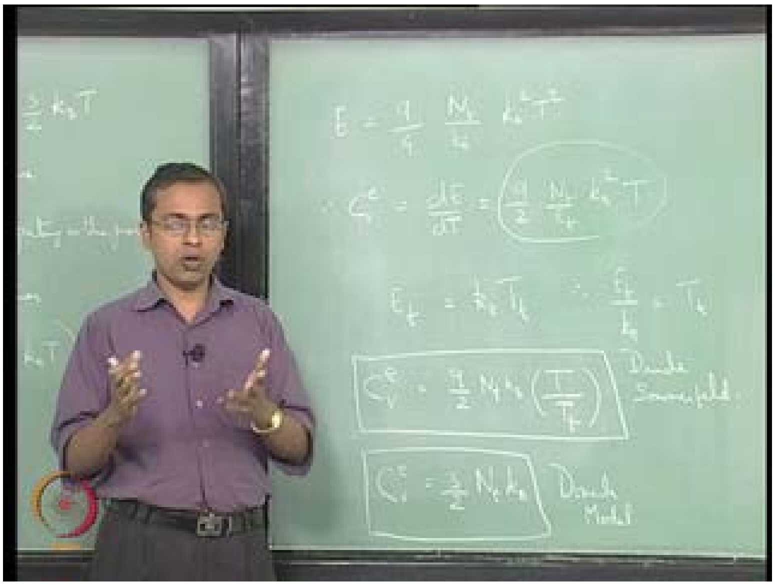

So, E equals what we just wrote down 9 by 4 N f by E f k b square T square. So, this is the expression we have, where this is the Fermi energy; this is the total number of free electrons per unit one. Therefore, c V E the contribution the electronic contribution to specific heat at constant volume is D E by D T and that is simply 9 by 2 N f by E f k b square T. So, this is the expression that we have. So, we have actually again emphasize we should always keep in mind that this is only the electronic contribution to the specific heat; this is not the total specific heat of the solid. You make a measurement for the specific heat of the solid; this is not the value you will get.

If you can isolate the electronic contribution to the specific heat that is the value you will get. Because there is lot of other constituents in the solid, which we are ignoring current calculation. So, that all the items of represent are all being ignoring and all the other electrons which are bound electrons there also being ignored. So, entire system is now much very specific system that we are looking at. So, this is what we have. Now, this is an expression that has few terms here; we will actually simplify this a little further. We noted in the last class so that specifically, we looked at Fermi energy, Fermi surface and Fermi temperature; these are all things discussed in previous class. In that we specifically said that, the Fermi energy E f can be equated to a Fermi temperature T s with this expression.

Just the way to have to k b T for the energy contributions at approximately k b T has the energy contribution at a temperature T. We will say that, this energy can be equated to some temperature T f; so that is this T f. Therefore, E f by k b is this Fermi temperature T f. If you look at our expression here we have the inverse of this; we have actually k b square but, if we just take it as k b times k b; we have a k b by E f here. So, k b by E f and another k b T are sitting there. So, k b by E f is there which an inverse of this is.

So, we can replace k b by E f as 1 by T f. So, this is simply c V E is 9 by 2 N f k b T by T f. So, 9 by 2 N f, N f is still there; one of the k b was still remains; so N f k b will remain; this T is still here. So, the other k b by E f is being replaced by 1 by T f. So, that is what we have got here. So, so what we have here is the electronic contribution to specific heat, some constant number of free electrons per unit volume times the Boltzmann’s constant; times a ratio of two temperatures, one is the temperature that the system is at so, we have moved at to; so if we are talking of you know few 100 Kelvin that is the kind of temperature we are talking of here. And this is the Fermi temperature T f, which is defined for a system. Now, when we also look that the Fermi temperature; we have we have some particular values for Fermi temperature; we will we will look at that in just a moment. So, this is the expression; there is some approximation made in this this is not the most rigorous expression that you can get, but in principle, this is the expression that you will get with respect to the Drude Somerfield model. A much more rigorous expression can be derived with where some of these constants will change lightly. this But in principle, this feature we will show up. So, this T by T f and other things will show up. So, a much more rigorous expression can be derived derived, but or our purposes this is adequate. So, this is what we get from a Drude Somerfield model.

So, the Drude Somerfield model gives us the electronic contribution to specific heat as this particular expression. If you look at the original expression that we previously had, this was the expression for the electronic contribution to specific heat at constant volume as predicted by the Drude model. So, this is an expression and is basically the same expression that you get from the ideal gas behavior. So, Maxwell Boltzmann statistics is used. If you use Maxwell Boltzmann statistics then you are talking of an ideal gas a collection of particles that behave like an ideal gas. And then this is the expression that you would get; and this is what we derive in one of our appeared classes. In our present derivation, we have taken the Drude Somerfield model which has replaced the Maxwell Boltzmann statistics by the Fermi Dirac statistics. And then we have come up with a lot of features associated which that replacement; we have seen all those features which is the Fermi energy, the Fermi surface, the Fermi temperature and so on. And relative to that, this is the expression we have got for the specific heat at constant volume. What we said also is that experimentally, if you measure this electronic contribution to specific heat, this is this is the measurement that you can in in in practice; this is mostly done at very low temperatures typically in the range of 0 to 1 Kelvin. So, that is the temperature range at which this is a more significant contribution relative to the contribution of the rest of the material.

Even at much higher temperatures, this can become a significant contribution. So, in most intermediate range of temperatures that we will measure, you will only see the contribution of the other constituents of the solid in significant quantities. So, in experimental sense typically, low temperature measurements are being made to get this electronic contribution to specific heat and of the order of m. Those are really low temperatures; those are no tends of degree or 0 degree c; there we are looking at minus close to minus 273 degree c effectively 0 to 1 Kelvin. So, that is the temperature range where you make this measurement. So, that is how you would experimentally get it; experimentally when it is determined, it is found that this expression here the Drude model prediction for the electronic contribution to specific heat at constant volume is larger than what is experimentally measured by a factor of 100. So, the order of two orders of magnitude, this value is higher than what is measured. Now, let see if you look at the new expression that we have got for the Drude Somerfield model, you will find this N f k b shows up in both of them. Therefore, this is more or less the same as before we have some constant up here this is 9 by 2 this is 3 by 2, but that is not a very significant thing. They are the same order of magnitude anyways. So, this much is essentially the same; so what is really different is this T by T f; so T by T f is the new thing that we have introduced effectively in or prediction through the Drude Somerfield model.

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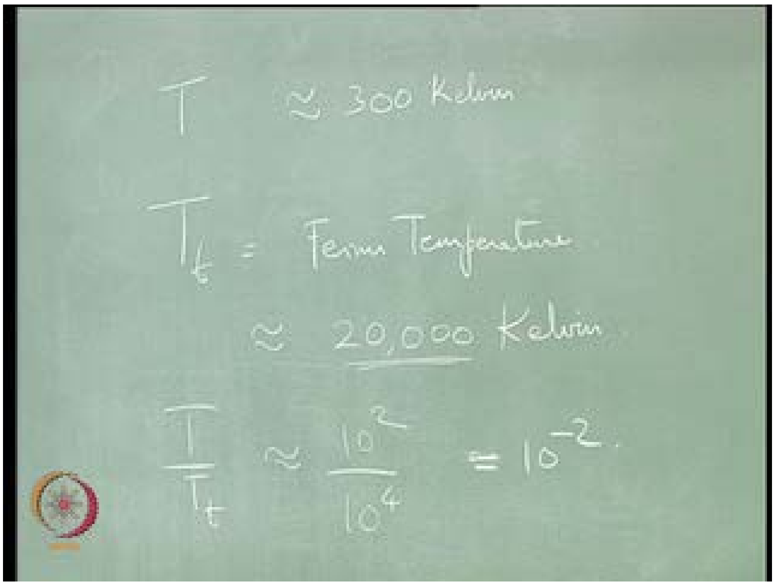

$T \approx 300$ Kelvin

$T_f =$ Fermi Temperature

$\approx \underline{20,000}$ Kelvin

$$\frac{T}{T_f} \approx \frac{10^2}{10^4} = 10^{-2}.$$

So, we will just need to look at this value of T by T f a little bit, if you look at T; if you looking at room temperature for example, this is of the order of 300 Kelvin. And T f is the Fermi temperature, if you look at the Fermi energy that most of typical metallic systems; if you look at the Fermi energy that they will have; if you do the calculation given a the given that we know what is the approximate number of a free electrons per unit volume; if you do the calculations and so on. Given the Fermi energy, if you calculate the Fermi temperature corresponding to those that Fermi energy we find that Fermi temperature is approximately of the order of say 20,000 Kelvin of this order.

So, 20,000 Kelvin is Fermi temperature that can be attributed to the Fermi energy in in typical metallic system. So, if you simply take a ratio of these two, so T by T f is therefore, that is of the order of 10 power 2; this is of the order of 10 power 4. So, this is of the order of 10 power minus 2 so this is of the order of 10 power minus 2. Simply, T by T f gives us 10 power minus 2 as the ratio of the two of them. And that is all the difference that we are really looking at, we said that the Drude model over predicts the electronic contribution to specific heat by factor of 100 and we have now got an expression through the Drude Somerfield model which is adding one additional term T by T f into the equation. And we find that the ratio of T by T f is such that is of the order of 10 power minus 2. Therefore, if this is of by a factor of 100 you multiplying it by 10 power minus 2; so you are now in the right order of magnitude. Therefore, this is a we have successfully shown that the Drude Somerfield model actually takes care of one significant drawback that the Drude model have. One of the most significant drawbacks the Drude model has now been appropriately accounted by making the changes that the Drude Somerfield model introduced into that in fact Somerfield introduced into the process.

And therefore, the changes in expressions that were caused due to those fundamental changes in the system, that were introduced. So, therefore, till now we I showed you through diagrams why the two of them might differ in these predictions? Because the Maxwell Boltzmann statistics says that, all the electrons can participate in the process. So, that is why the energy associated with that process is significant. Drude Somerfield model using Fermi Dirac statistics says only electrons close to the Fermi energy can participate in the process. That is essentially the difference in this calculation is this calculation.

Here, we specifically accounted for all those number of electrons close to the Fermi energy and within k b T of the Fermi energy is said, they can participate in the process. And then we looked at the density of states of the Fermi energy multiplied by the factor 3 by 2 k b T, which is the amount of energy associated with each electron. So, it taking all that into account we arrived at this expression. So, we find that in fact, if you look at how everything has turned out seemingly the the specific factor introduced by the Somerfield model which is T by T f specifically, takes care of this problem and solves it to our satisfaction. It gets us into the correct order of magnitude for this prediction.

And as I mentioned, in this kind of analysis getting us into the correct order of magnitude is something that is very valuable to us; is something that we then accept. So, of course, as we have already seen with the Drude model sometimes, you can get into the correct order of magnitude with two errors cancel account. So, that is not something; that is useful to us and so this takes into account of all of that, and gets us simply correct order 9 by 2. So, once again I will just highlight this fact, when I mention this earlier; this is a very larger number 20,000 Kelvin.

So, we need to understand that, this does not mean that your material are sitting at 20,000 Kelvin clearly, we are talking of a material sitting at room temperature. So, 300 Kelvin or of that order, it is started from 0 Kelvin; you raise the temperature two or few 100 Kelvin. We are simply saying that, in that material you have a lot of atoms; you have a lot of electrons that are bound to those atoms; all of those are at around this temperature and they represent a very significant thermal mass. So, then amongst the free electrons also you have electrons which are at very relative low energy going up to higher and higher energies.

The Fermi energy is simply the highest energy occupied by very small fraction of electrons present within the system; or at least it is very small fraction of electrons present within the system; it is also an extremely tiny amount of the thermal mass of the system; which is what is sitting at that at that energy level. And as a distribution therefore, it is at the tail of the distribution or the leading edge of the distribution. And that extreme end of that distribution alone sitting at, if it can be is sitting at some energy which if it can be converted to a temperature would correspond to this temperature. So, that is the sort of the frame work within which we understand the fact that the Fermi temperature is 20,000 Kelvin.

It is like saying that within a within a material sitting at room temperature, there is an electron sitting at 20,000 Kelvin. If this lose piece speaking that is the wave we would like to rationalize the fact that there is a twenty thousand Kelvin temperature in this system. So, this is what it is but, given that this is twenty thousand Kelvin; and this is consistent with the Fermi energy of the system T by T f works out to 10 power minus 2 which solves all our problems. So, to summarize where we have come so far; we have looked at the Drude model identified problems with it and systematically solve them using the Drude Somerfield model. And what we have done today is a demonstration that numerically we can see that the Drude Somerfield model has succeeded in a much specified example where the Drude model fail. So, this is the success that we have here. So, having come this far we understand that, we have made an improvement Drude Somerfield model has an improvement. So, it is therefore, necessary for us to stop and consider what the further scope for improvement from this model is? What are issues that perhaps even this model is not really addressing? If you look at it from that perspective, what you see is that the Drude Somerfield model is actually still using certain basic ideas of the original Drude model, which is that it is a free electron gas.

And it also says that you know other things are all equally, it is not significantly looking at least in the in the extent that we have developed it so far; it has not significantly looked at any of the impact of the details of the material.

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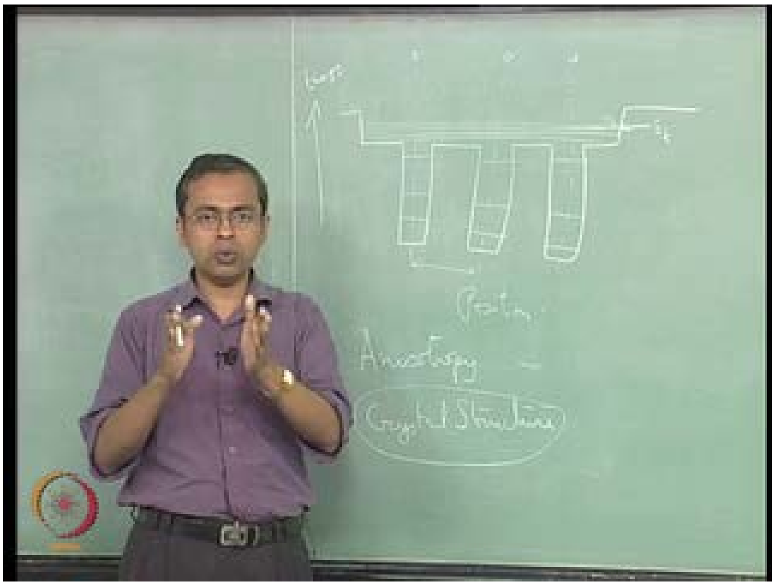

So, for example, we made this diagram saying that the distribution of potential within the system is in a in a solid can be described with a diagram that looks something like this. So, this would be energy; this would be position and these are the positions of the ionic cores. So, these are the x-coordinates of those ionic cores and these are the bound electron energy values. So, this is what we have and this is what the Fermi energy is.

So, this what we have, when we looked at the contribution to specific heat, we are basically only looked at the top most layer of this entire collection of electrons; this top most layer how it is participates in specific heat process. So, that is what we have looked at. Now, in terms of other properties say electronic properties and so on. In principle, we have not really changed a whole lot from a respect to how the process is occurring. One of the issues that we still have in our description is that, if you look at a typical solid; you take any material let say any metallic systems silver, copper and so on. In most metallic systems if you take a single crystal of that solid; single crystal meaning from one end to the other end, all the planes or in perfect atomic order. If you take a single crystal of the solid we discuss the solid that when you measure properties across the single crystal, you will find that based on the direction in which you are measuring the property the property can change significantly. Classic examples in fact for example, something like carbon where you can have of course, that is not exactly metallic, but if you look at carbon; you can find that you know it has a structure whether a planes of carbon atoms. Along the plane, the electronic connectivity is excellent; a perpendicular to the planes the conductivity is terrible. So, you can have it is more or less an insulator perpendicular to the planes; it is an elliptic conductor along the planes.

So, this is basically the term we use for this is an isotropic. So, an isotropy exists in many systems and can be very glaringly experienced or measure. So, it is not something that is not something that just settling thing that is minor correction that you need to throw in. The property can change by several orders of magnitude depending on the direction in which you measuring the property.

So, up and till now the calculations that we have done calculations that we have done have in no way captured the directionality of the property. So, nothing that we have done so far when we say number of free electrons per unit volume; that number of free electrons per unit volume is the same regardless of which direction you are looking at because it is on a per unit volume basis and the per unit volume has no direction associated with it. So, it is a enough a simply the same number; the Fermi temperature is a same temperature. So, well more specifically, N f is the same value and therefore, you do not really have any variation in say the property in based on which direction you are looking at. So, what we need to consider for a moment? What is it that is inherent to the material that dictates that one direction is different from another direction? What is inherent to the material that is that dictates that any one direction is different from another direction regardless of how it is different is something that we have to consider. The thing that differentiates between directions is the crystal structure. So, the crystal structure now has there are crystal axis; there are angles associated with these axis; there are unit vectors associated with these axis depending on the material you are looking at.

So, that is very specific structural information that exists about the system. In our calculation so far, we have not accounted for the structural information in any manner. So, if you go back to this diagram here, the crystal structure information to speak even in a 1 dimensional sense. We have this diagram is drawn for a 1 dimensional solid; we will assume that we are still talking of a 1 dimensional solid. So, that our analysis is then consistent with whatever we have done, but at the same time more and more details are incorporated into the analysis. In this one dimensional solid, the crystal structure information is to speak comes from information on what is this facing so to speak.

These are the ionic cores; they are the ones that are sitting at those crystal lattice points. So, the crystal lattice is now decorated with these particular atoms or if you want to call them as atoms, or if not as ionic cores; those ions are sitting at those specific lattice points. So, the positions of these ionic cores therefore, represents in the crystal structure information. So, if you are saying that an isotropy is in some ways related to the fact that crystal structure is an isotropic with respect to different directions. So, if you look at spacing between ions in one direction, it is different from spacing between ions in another direction; the angles in which they are laid out are different and so on.

So, if the spacing is different and so on that the information is directly from the crystal structure which is directly being represented by these locations. Therefore, one of the things that we have to understand is what is the impact of these ionic cores sitting at these locations on the behavior of the electrons which are sitting up here? So far, we have actually separated this picture; so far we have said that these are nearly free electrons which are free to roam through the solid we have used and mathematically incorporated that information in different ways. But we are basically said that these are nearly free electrons, they are free to run across the extent to the solid and these are bound electrons which are bound to those ionic cores.

These are the energy levels corresponding to those bound electrons bound to these ionic cores. And we separated these two; we sort of said that this is independent behavior related to all of these. In fact, one of the assumptions that we made is that we kept saying that the potential is sort of uniform throughout the solid. There is no interaction; there is no we did not put in any detail for the interaction between these electrons and what the ionic cores in the environment system provided by those ionic cores. We simply said that we put in one averaged term for the resistive forces that the electronic speed as sense as it travels through the system.

So, we had actually neglected at any impact of these ionic cores on those free electrons. So, of course, as for calculation that is fine; you can always say that I am neglecting a certain effect and we are running a certain calculation. And to the extent, that we neglect at this we still have made very good predictions on a number of things. Several things were predicted correctly even certain errors we made earlier on we have been corrected those. Therefore, all that is fine, so what we are saying is that now this additional information that we see about the material which is the anisotropy of the material has somehow not been captured by whatever calculations we have done so far.

So, we find that that information comes from is already there in this picture in the locations of these ionic cores. Therefore, we understand that somehow the location of these ionic cores also impacts the behavior of these electrons. Only thing is we have not actually incorporated that process; we have not incorporated this detail into our system. So, what we need to do is, we need to understand and in our analysis since we are using the quantum mechanical description we can think of the electrons as particles or as waves. We would like to understand, what is the interaction of this wave like behavior of electrons with these periodic structure of ionic cores that is present in the system?

So, this is the direction in which we will (( )) in the next few classes. To do this, we would have to take a two-step approach. First we will look at the ionic cores and how they interact with waves in general regardless of whether the electrons waves and so on. So, we will look at them as how they interact with waves in general which is effectively the diffraction process, but not just that we are already using k vector so to speak the wave vector k is 2 pi by lambda.

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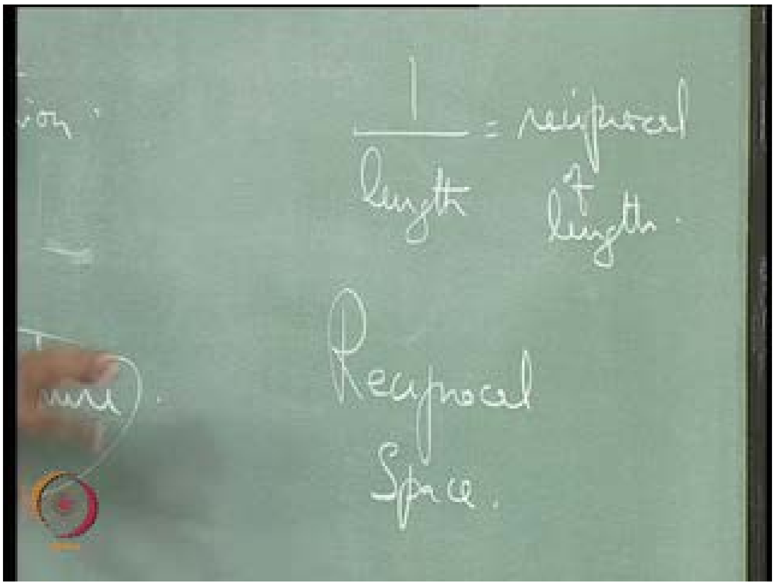

So, this is the wave vector corresponding to these electrons here. We will use similar one by length dimensions and in that context one by length dimensions simply reciprocal of length. So, we will look at the interaction of waves with ionic cores in a in a descriptive frame work which consists of the reciprocal of length such a frame work is referred to as reciprocal space. So, we will develop these concepts called reciprocal space; we will find how it relates to real space. So, we will see reciprocal space as a separate entity; we will see how it relates to that reciprocal space will now contain all this crystal structure information in reciprocal of length units.

We already understand how it might be in real length units. In the early cryptographic courses, that you would have seen that so we already understand crystal structure and real space, as we call it the normal x y z space. We will look at crystal structure and what it represents in reciprocal space; we will see how diffraction can be described in real space which we already understand and how the same description can be given to as a reciprocal space. So, we will understand reciprocal space from those prospective. Therefore, we will understand the manner in which the presence of ionic cores impacts or interacts with the waves present in the system within the description given to us by the reciprocal space. So, this we will learn as an independent process.

Then we will relate what we will do is having understood that as an independent process. We will we will take into account the fact that the electrons that are in the solid are showing as wave like behavior. And as far as the description of the diffraction process is concerned or the interaction between waves and the ionic cores is concerned, it does not really matter where the wave is coming from whether it is being an externally introduced into the system or it is something that is within the system. Therefore, we will be able to extend our analysis of reciprocal space and diffraction processes within from this frame work, where we are just talking of independent set of waves interacting with a periodic structure which is what we will find under reciprocal space.

That description and that discussion and the results that we get there can be extended and directly incorporated into a situation; where we are looking at the interaction of these waves with this periodic structure. That is all the information that we want we want to know, what is the impact of this periodic structure on the behavior of these waves that are of their so to speak in energy level. When we do that we have incorporated the periodicity of the structure into the picture that we have described and the picture already has many other details; which are right taken together this periodicity of this structure plus all the wave description of that of the electrons that are in the system.

We will have much more complete picture of the solid with the significant amount of detail of the solid which now incorporates even its crystal structure. Presumably at that point, we will now also be able to see the anisotropy of the behavior of the phenomena that we are examined. Therefore, in the next class we will head off towards our discussion of reciprocal space and it will it will look like a separate discussion atleast initially till we will come back, and we put it back into this picture; and add on add on all of these details; and then see what is the impact of the reciprocal structure on that on the electrons that are moving.

So, in this direction, that we will proceed before we get an even better even better and much more improved understanding of the system from a theoretical prospective. So, we will halt here today and we will take it up in the next class.