Condensed Matter Physics
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Lecture – 26
Band Magnetism; itinerant electrons; Stoner model

We have seen so far how the exchange interaction between localized electrons spins leads to ferromagnetism and other form of magnetic ordering as a result of the Dirac Isenberg exchange interaction.

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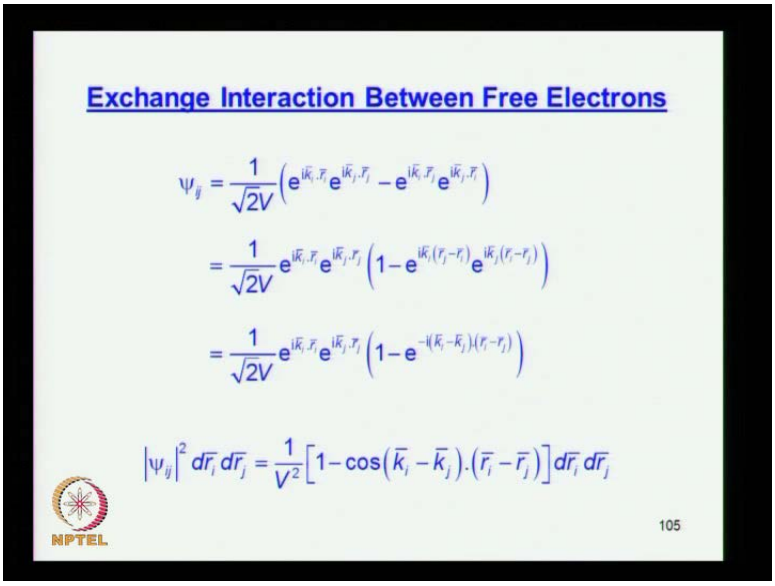

But of course, this is somewhat not our going to limited interest, because we know that the well-known ferromagnets do not have localized spins.

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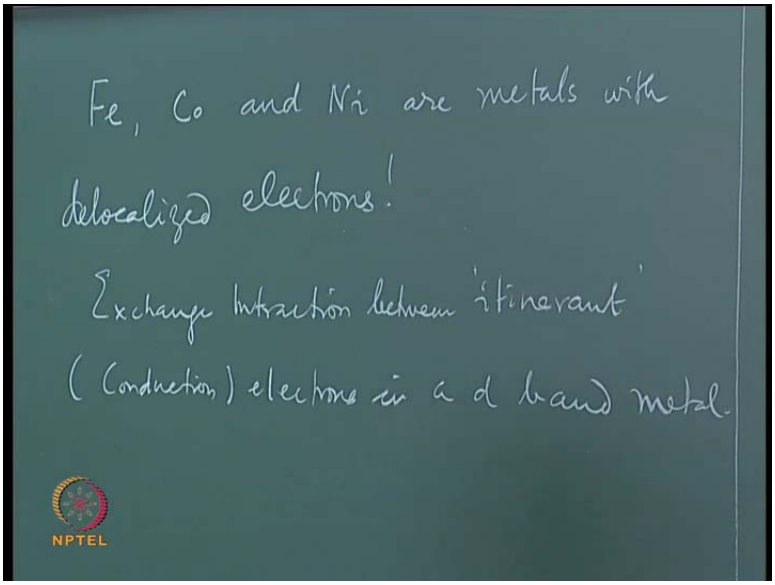

Namely the ferromagnetic metals, such as iron, cobalt and nickel are metals with delocalized, not localized electrons. So in order to account for the ferromagnetic ordering in these metals, it is necessary to consider exchange interaction between itinerant or conduction electrons in a d band metals. We can use the same concept that we consider for the exchange interaction between a pair of electrons and build in the idea of the electron wave function for itinerant electron.

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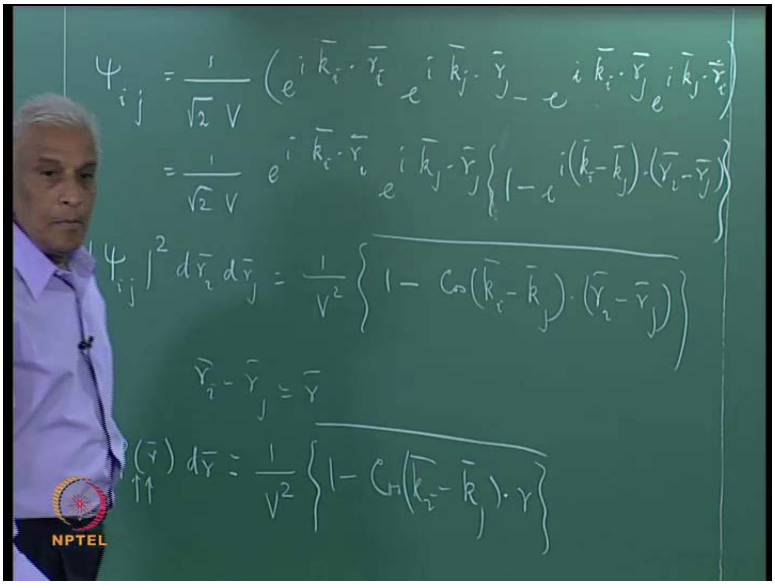

So we can write the effective wave function for such a pair of electrons i and j as one by root two V e to the power i k i r i e to the power i k j dot r j minus e to the power i k i dot r j e to the power i k j dot r i. This is the positions at r i and r j, the electrons at r i and r j and wave vector k and k i and k j. Now this is the exchange because of the in disguise visibility of the electrons this is the exchanged term and the two electron wave function should be anti-symmetry with respect to the spatial part in order to give raise to a ferromagnetic or spin parallel wave function.

So rewriting this, we can write this as into one minus… Therefore, psi i j square, mod psi i j square dr i dr j will be from this, we can easily see that this will have the form taking r i minus r i j as the separation r between the two electrons. We can now write the probability for two spin being parallel, two electrons spin being parallel, and being separated as just this. Now this should be multiplied by d r here, and this will giving you n up.

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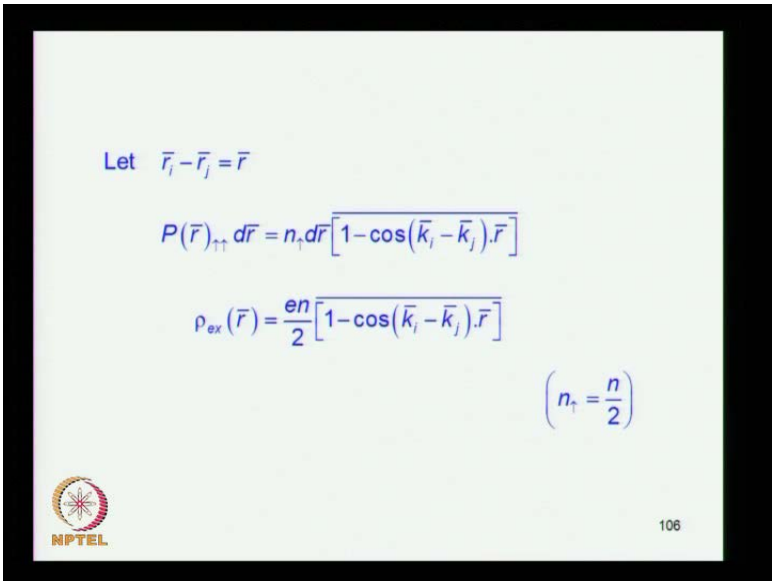

Where n up is the number of electrons spins.

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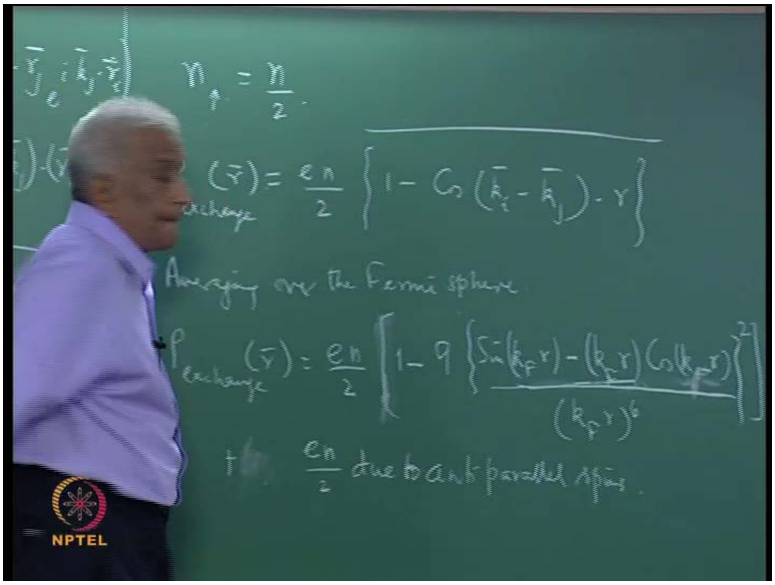

In this spin up sign band which is equal to n by 2, so that using this we can write this exchange charge density as by multiplying the electronic charge and… We take this average, this dash, this dash over this form – bracketed term is just the average, now we average over the Fermi sphere, so that we have rho exchange over r as.

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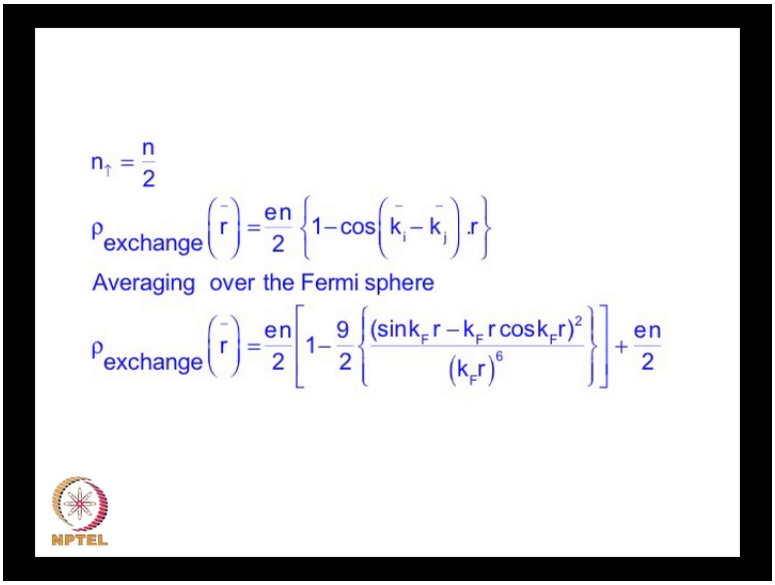

So that would be the form of this exchange charge density. Now to this of course, we must add the charge density e n by 2 due to anti parallel plus the charge density, due to anti parallel spin.

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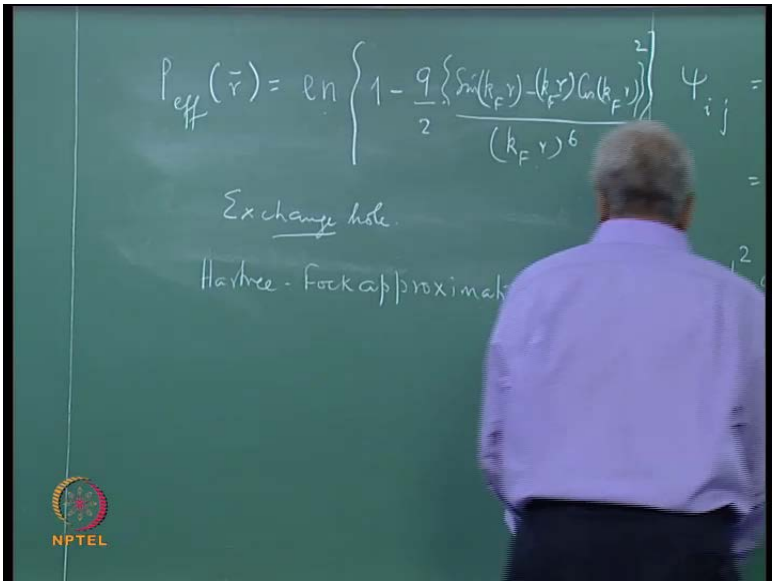

Doing this, we finally arrive at the effective charge density as…

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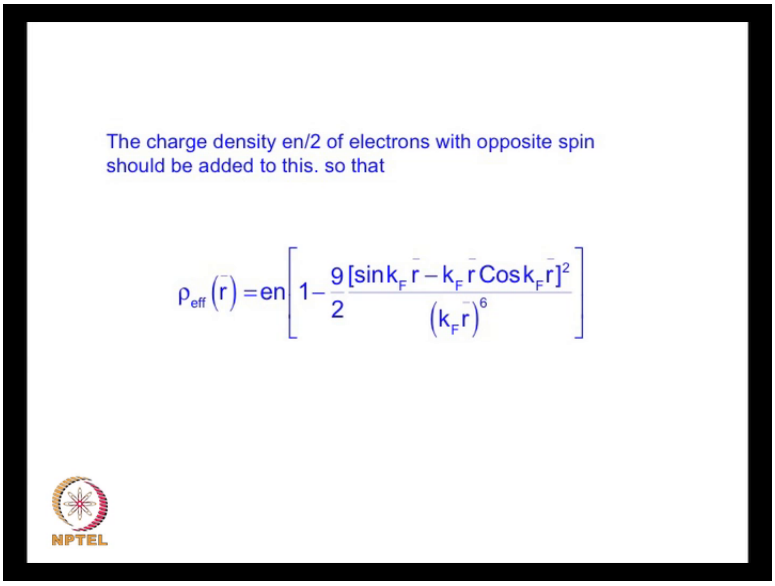

So that would be the form of the effective charge.

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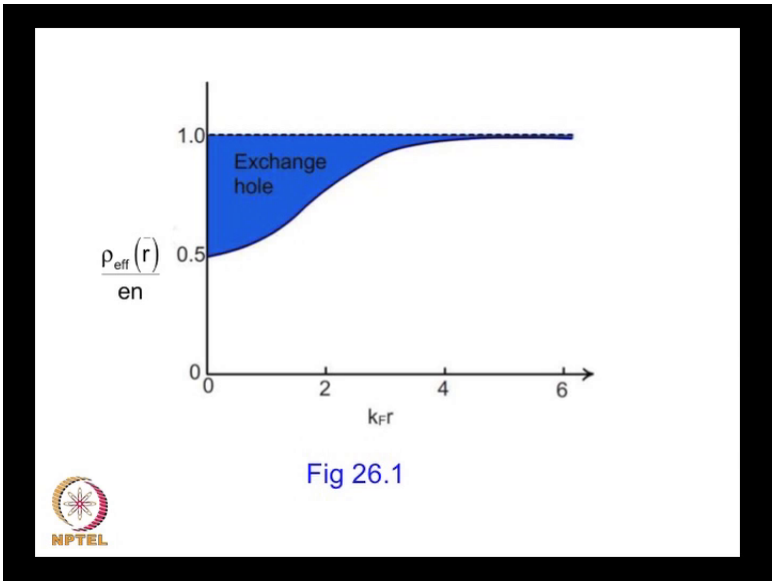

And this is shown in the form of a plot of this effective charge normalized by e n versus as a function of k F r and that shows so called the exchange hole. This means that the presence of the exchange interaction leads to a situation where the effective charge density is reduced because of this exchange correlation.

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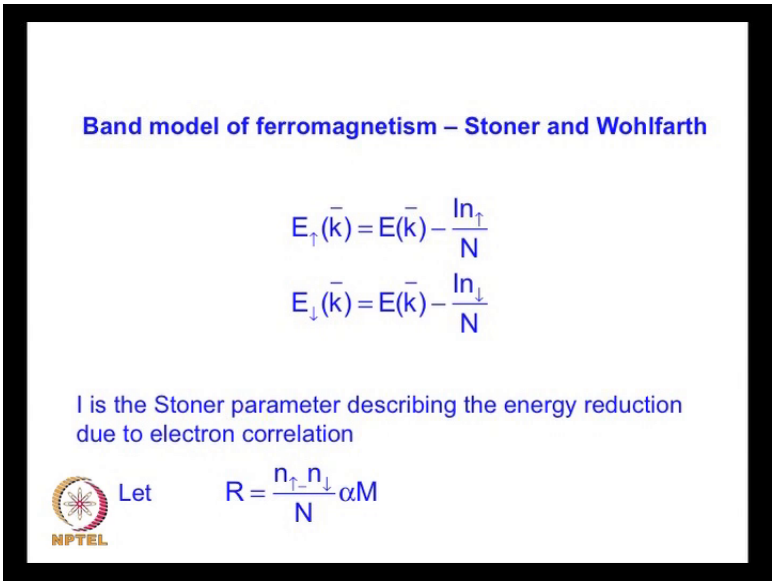

So this leads to a renormalization of the electron energies, which is the stating points of the Hahree -Fock approximation.

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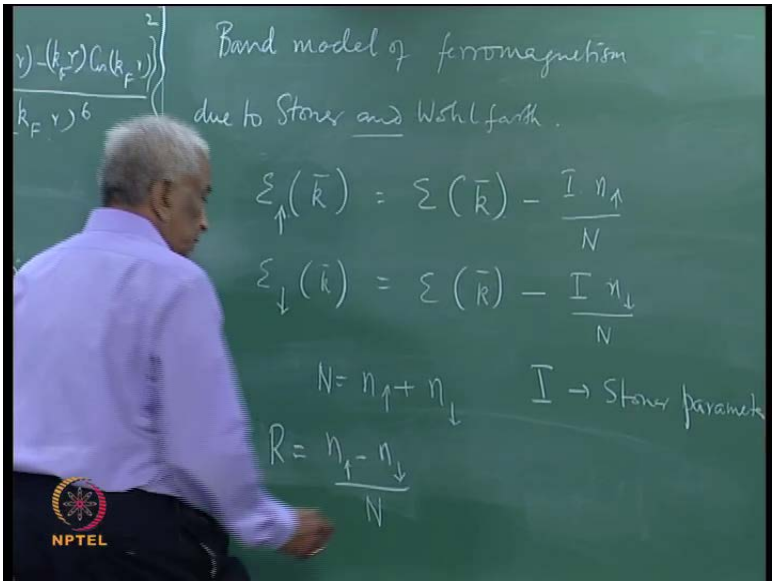

We will not go into details of this, but use this idea to discuss the so called band model of ferromagnetism. This was first proposed by Stoner and Wohlfarth, effectively that means that the energy of the electrons in the spin up band and in the spin down band can be written as basic original energy minus I into n up divided by N, and this is minus I down by N. Where N is of course, n up plus n down that is the total number of electrons, and I is the Stoner parameter, which describes the energy reduction due to electron correlation. We define a parameter R which is n up minus n down by N. So this is the difference between the number of electrons with up and down spins and therefore, this should be proportional to the magnetization. In order to put this electron energy, which we have written in a slightly more transparent form, we redefine the zero of energy with respect to by subtracting.

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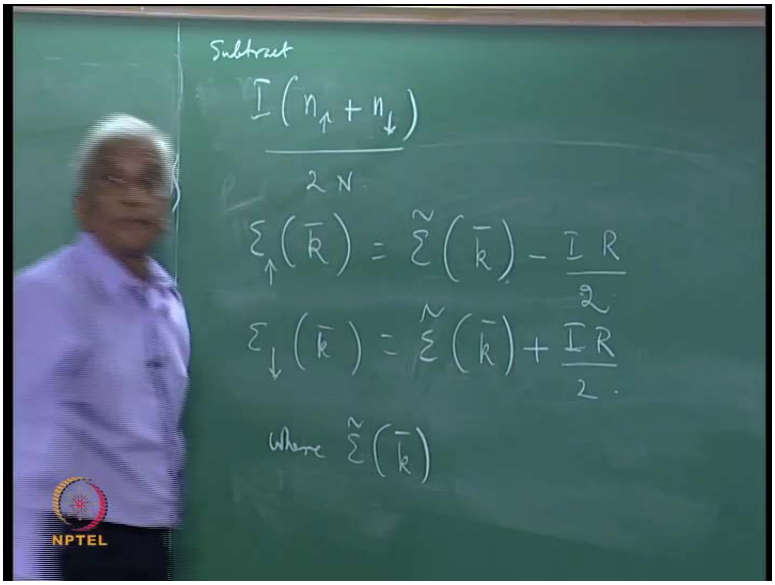

I times n up plus n down by 2 N, so subtract, this from the energy. And redefine the energy, so we denote this by e tilt minus I R by 2. This can be easily verified and similarly e down turns out to be given by…

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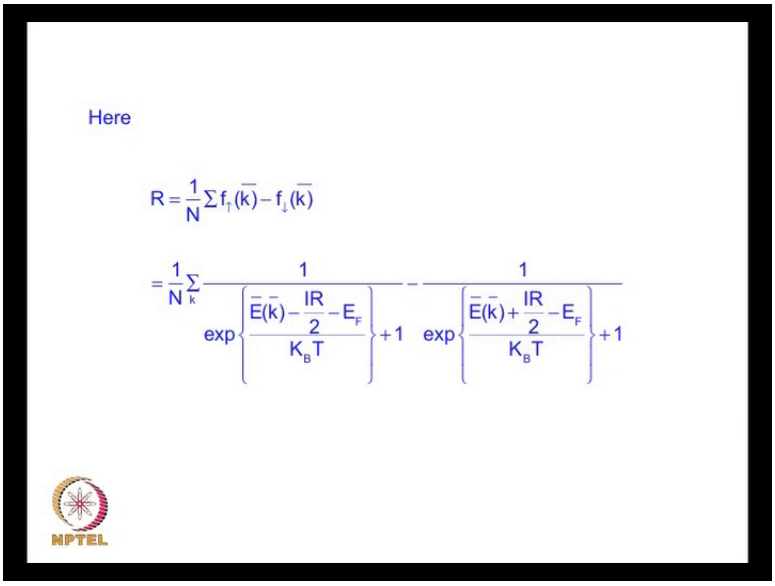

Where e tilt of k equals e of k minus this quantity. So starting with these, these are the renormalized electrons sub band energies and our aim is to calculate the magnetization, which is

proportional to parameter R. So we can write R as 1 by N sigma f up k minus f down k the summation over, all k values, where f k is the Fermi Dirac distribution function which we have discussed already. So substituting for this, R turns out to be one by N sigma over K writing the actual form of the Fermi Dirac distribution function and substituting for e up and e down values the energies. So this will be e minus e tilt minus e F minus I R by 2 by k B T, because there is a negative sign there plus 1 minus 1 by…

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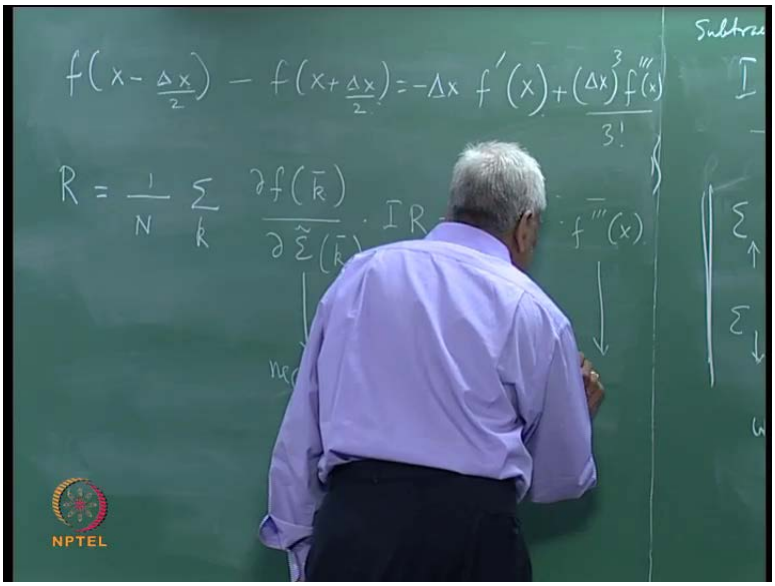

So we simplify this by noting that we have a function f of X minus delta x here, and the function with f of X plus delta x. So this is given because of the exponential, we can write this as plus higher order term involving delta x cube into f x by 3 factorial etcetera. So using this, and applying it to this, we get the parameter R as 1 by N sigma K d f k by d e k times I R, neglecting the other terms, which is necessarily positive, the times f dash. So this is we know the Fermi Dirac distribution function has a negative sign here, whereas the next term involving the third order derivative is positive.

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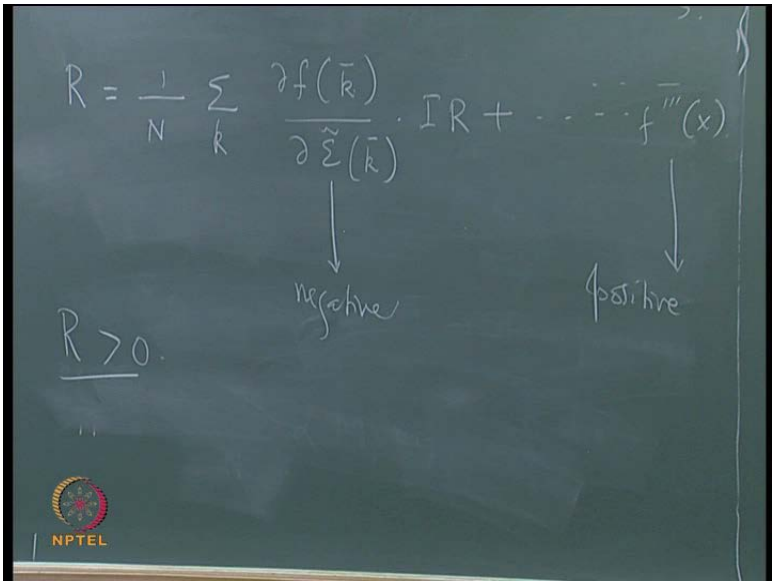

So if we want a positive magnetization, a non-zero magnetization, which means that R should be positive. We arrive at the Stoner criterion for ferromagnetism, we can see readily from this, this criterion to be…

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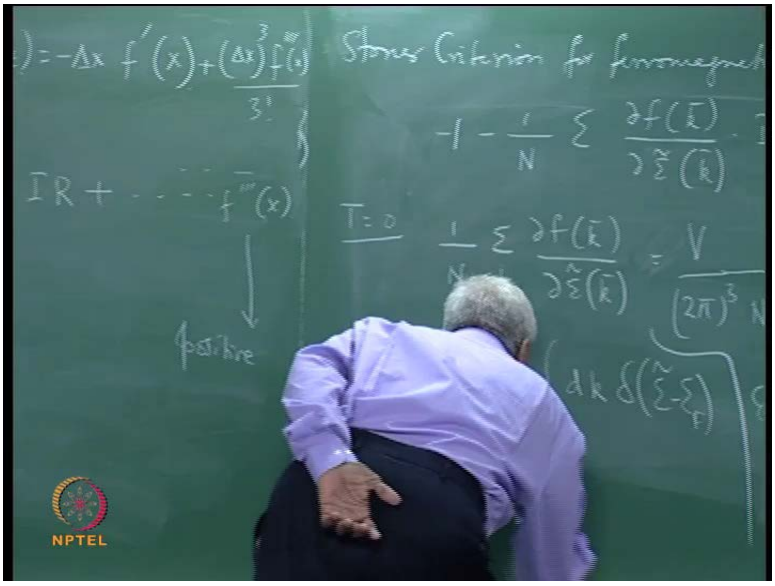

This will have a maximum value at t equal to 0, and it will have a particularly simple form at absolute 0. So you will evaluate this at absolute 0 over the summation can be written as… And

we know this is going to give you a delta function, therefore, we can simplify this as… So that would become, where D of e f is the electron density of states of the Fermi energy.

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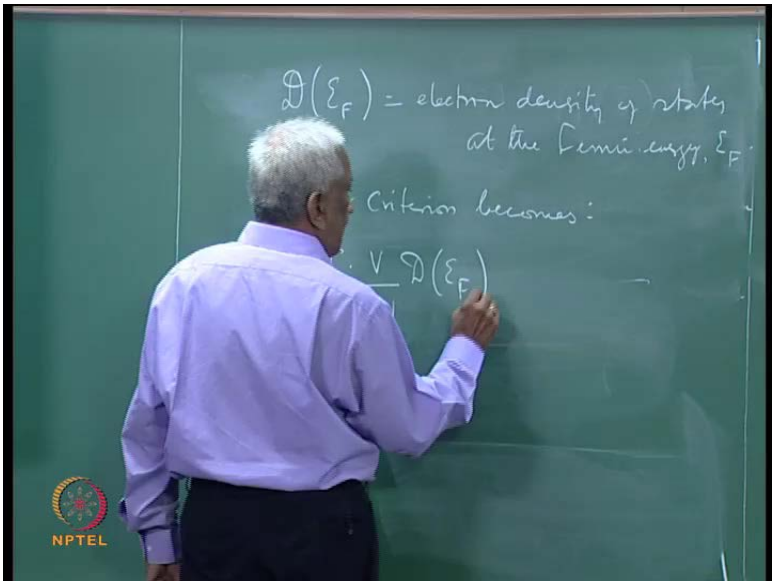

So from this, we get Stoner criterion as…

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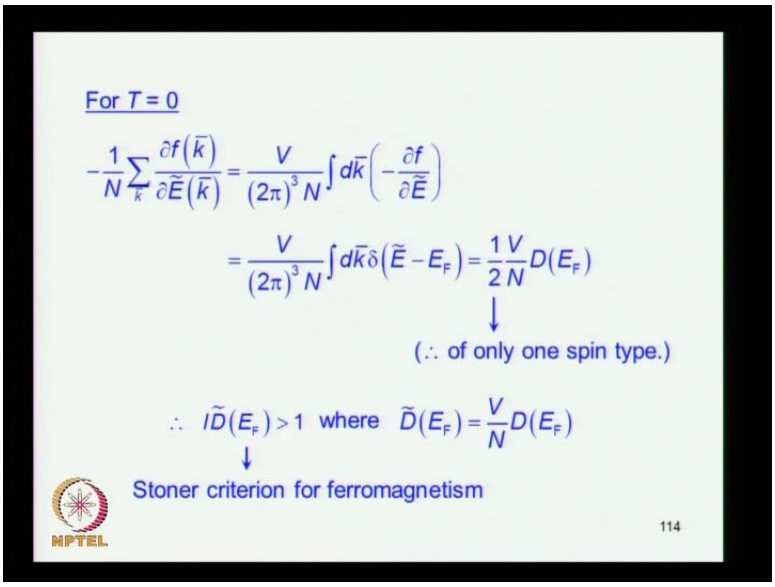

And we can redefine V by 2 N D of E F as some D tilt of E F, in which case we get particularly compact form for this Stoner criterion for ferromagnet. Now this has been calculated, the

electronic density of states at the Fermi level for the various metal have been calculated and using these values, the product I times D tilt of E F can be calculated and that is shown in the picture.

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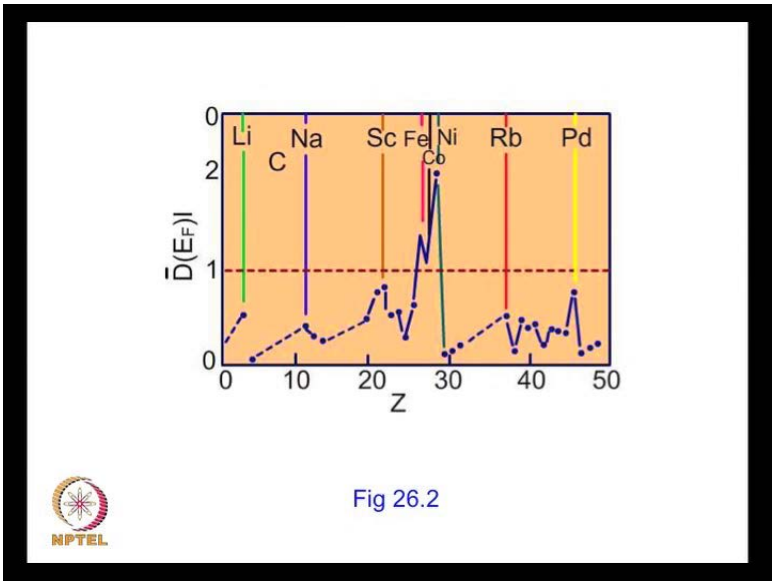

And it can be seen that the Stoner criterion is fulfilled only for iron, cobalt and nickel, so that is a very remarkable result predicting ferromagnetism according to the simple Stoner criterion in D band metals namely iron, cobalt and nickel, which are well-known to be metallic ferromagnets.

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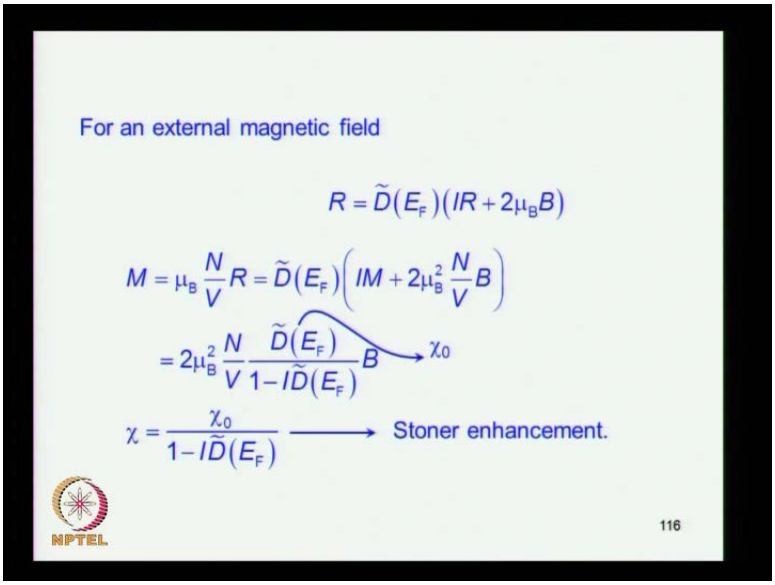

So that is how this simple Stoner model accounts for ferromagnetism in these metals.

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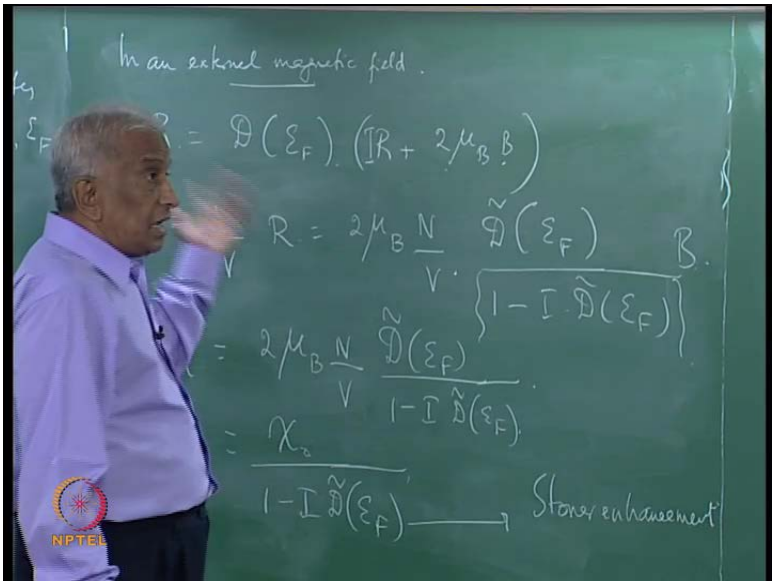

Now the next question is what happens in an external magnetic field. It is quite simple and straight forward, so this Stoner parameter the R becomes… Where this is the two mu B B is the Zeeman splitting in the presence of the applied magnetic field. So instead of I R, it becomes I R plus two mu B B and the magnetization is nothing but N by V times R. So that can be written

straight a way in the form, so the magnetization therefore we get the magnetization is given in this form in the presence of an applied field. Therefore, we can define the susceptibility as the ratio between M and B which is given by, so it has the form chi 0 by 1 minus I times D tilt e F, so this is known as an enhancement factor, this is called a Stoner enhancement of the magnetic susceptibility. So this is the Stoner enhancement factor, which increases the magnetic susceptibility.

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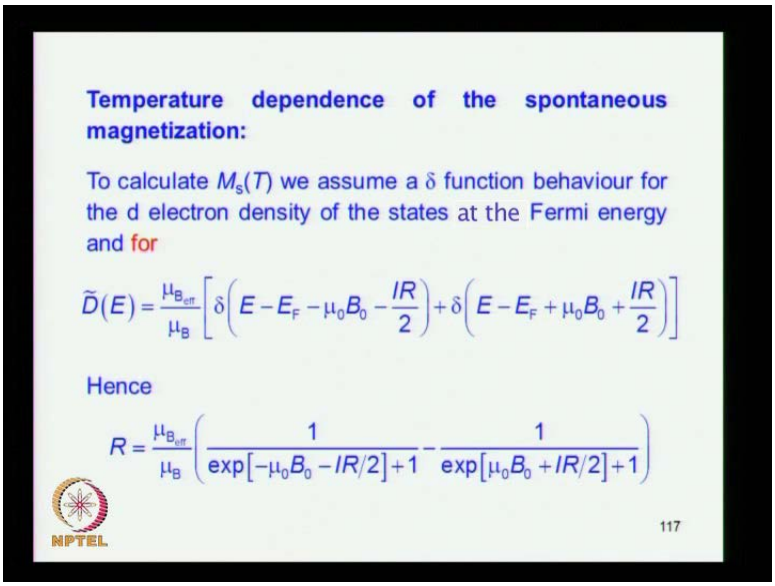

Next, we would like to calculate the spontaneous magnetization and its temperature dependence.

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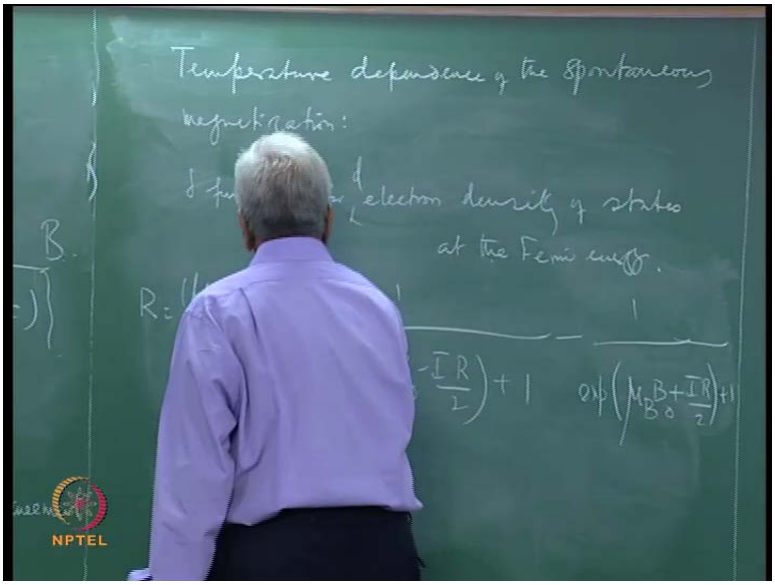

You know to calculate this, we assume a delta function behavior for the electron density of states, D electron density of states at the Fermi energy. In order to keep the calculation simple and with that assumption, we get the parameter R as we have same as before exponential mu B B naught minus I R by 2 plus 1 minus 1 by exponential mu B B naught plus I R by 2 plus 1. We set to bring it to a simpler form, we make the following substitution, we set T c, a parameter T c as I and mu B effective by mu B into 4 k B.

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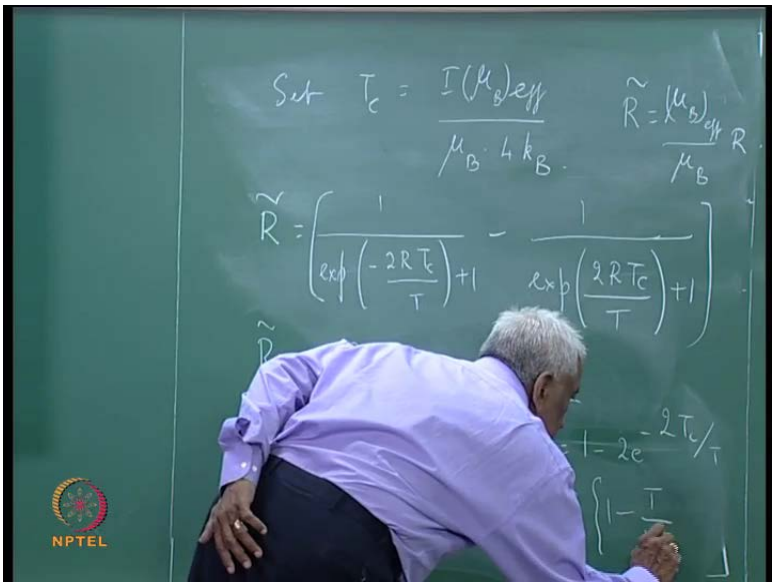

We also take R tilt as mu B effective by mu B times R, so that in terms of this, the R tilt becomes simply 1 by exponential two R T c by T plus 1 minus… This shows the correct behavior, this tends to equals to 1 for T equal to 0 and equal to 0 for T equal to T c. So T c defined in this way is the Curie temperature of this ferromagnet. In addition for T very small compared to T c, it is well below the Curie temperature, this R tilt is given by 1 minus 2 e to the power minus 2 T c by T. And the neighborhood of T c, this is given by root three times 1 minus T by T c.

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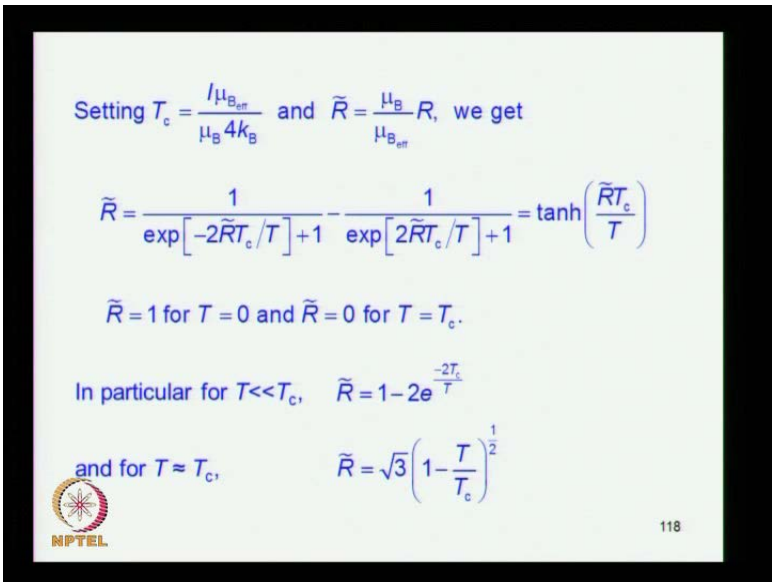

So this gives a number of things to compare with experiment, the figure shows the factor parameter R tilt as the function of T by T c.

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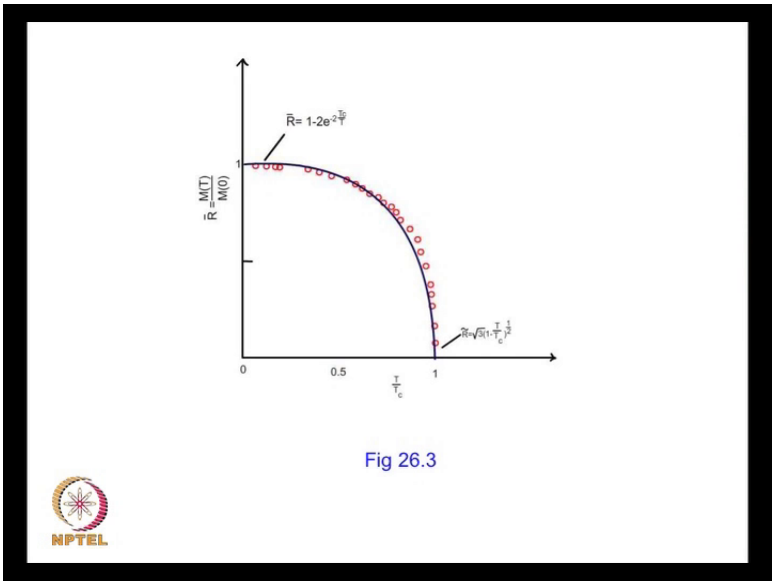

So this is the near the critical temperature, the expected behavior according to this model is root 3 times 1 minus T by T c to the power half, giving rise to a so called a critical exponent of half. But what is experimentally observed is one-thirds has can be seen from the next figure.

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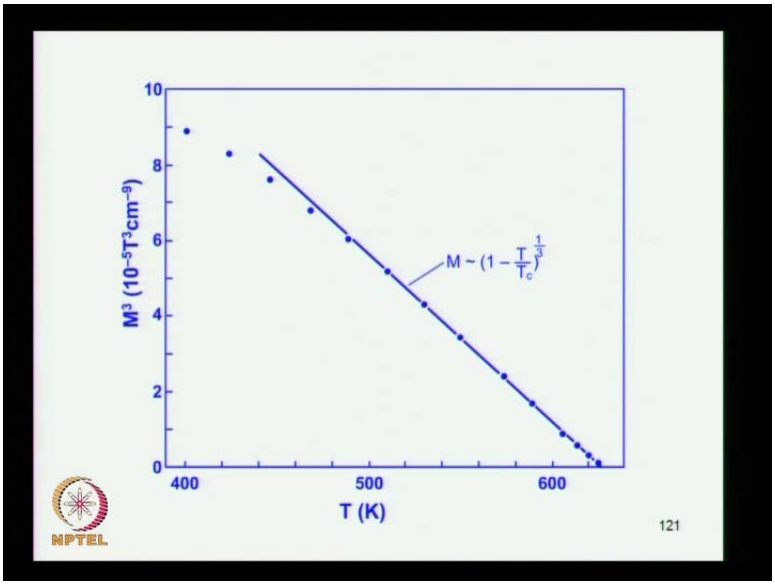

So the critical exponent magnetization goes as one minus T by T c to the power one-thirds in the neighborhood of the critical temperature, so there is a strong deviation in the critical behavior at

the ferromagnetic Curie temperature. Also the low temperature behavior, there is considerable deviation of the experimental results data points from the expected theoretical curve.

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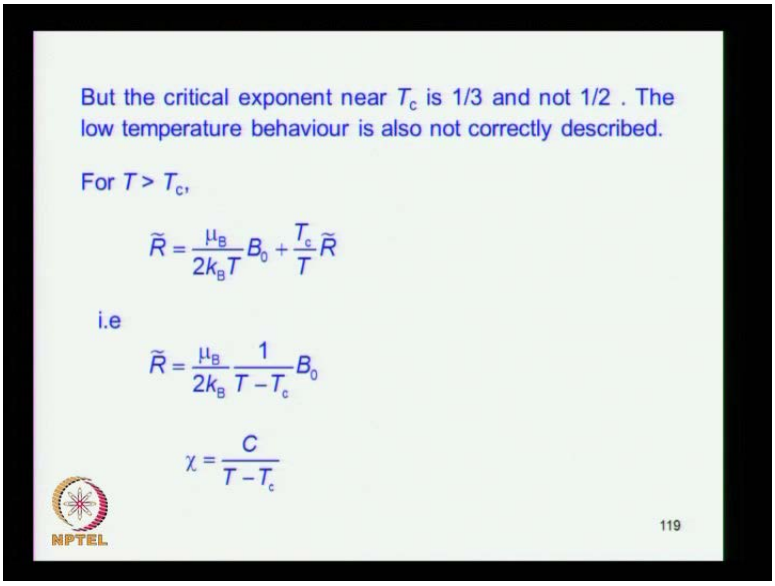

So these are due to the shortcomings of the Stoner model, especially that gives Stoner model does not take proper account of the excited states. Because in addition to spin flips, a cumbering the excitation from band to another, other element excitation with a smaller quantum of energy or possible and they can also cause spin flip.

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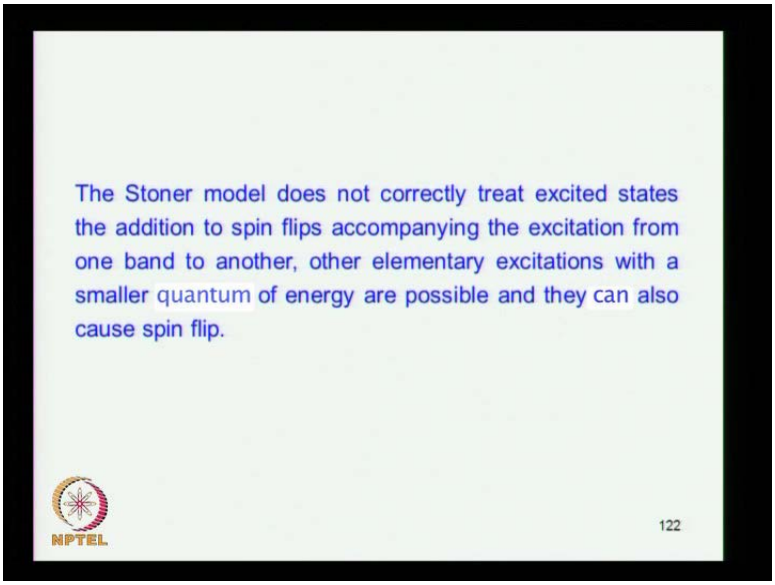

This is not taken into account in the Stoner model.

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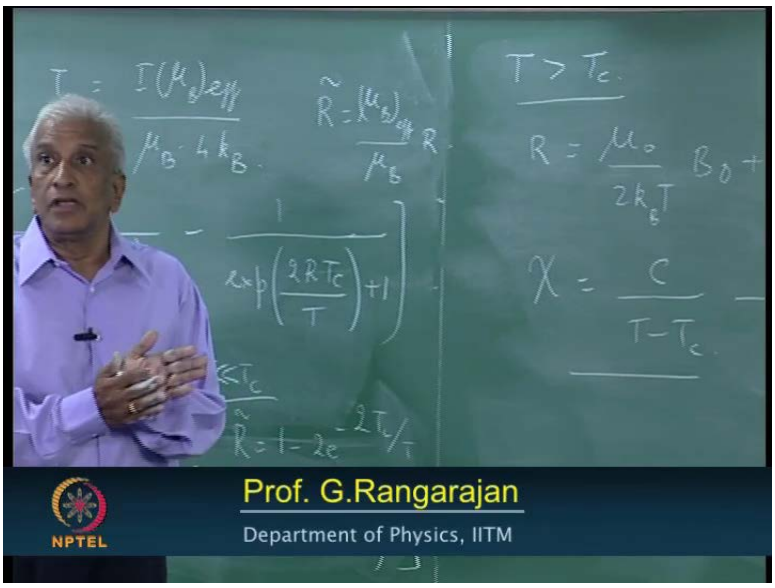

Now for T above the Curie temperature, T greater than T c, we can expand the exponentials and write R as mu B by 2 K B T into B naught plus T c by T into R, so that is leads to a susceptibility which goes as C by T minus T c. And this we can readily recognizes as the Curie Weiss behavior. So in short, we have described in terms of the simple Stoner model, how one can

account for ferromagnetism in a d-band metal, such as iron, cobalt and nickel and how this leads to features, which predict the correct Curie Weiss behavior and also leads to a Stoner enhancement of the susceptibility.

The temperature dependence of the spontaneous magnetization of course you have the correct overall behavior for the order parameter namely the magnetization, but the critical behavior as well as the low temperature behavior are not very well described by Stoner model, because of the improper treatment of the excited states. So with we have some idea of how band of model of ferromagnetism can be used to describe magnetic ordering in metals. With this we conclude our discussion of magnetism.