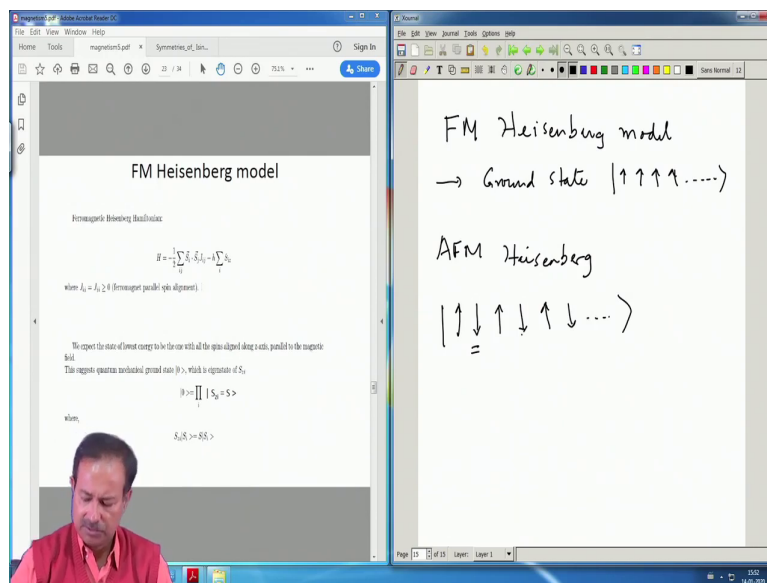


Electronic Theory of Solids
Prof. Arghya Taraphder
Department of Physics
Indian Institute of Technology, Kharagpur

Lecture – 46
Ground State & Magnons/Excitations

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Hello and welcome. We have shown so far that the ferromagnetic Heisenberg model; Heisenberg model has a ground state model, has a ground state which is all spins up. If there is no there is no magnetic field of course, I could also choose all spins down. So, magnetic field actually chooses a direction, but nevertheless this is the ground state, this classical state the intuitively correct state is the quantum mechanical ground state as well.

And then I mentioned that AFM Heisenberg model, AFM Heisenberg model is not so easy, the trouble comes we do trouble comes from the fact that the intuitive state which is this is not even an eigenstate and that is because if you operate by S^+ on the these spins then it will not be 0. So that means, that you that Hamiltonian that I wrote down operating on this will not return the same state even.

So, this will become up that means, a different state. So, that is the big problem and that problem is insurmountable, almost insurmountable. And that is the reason we cannot solve

Heisenberg model analytically except in one-dimension where it was solved that solution is of course a very famous solution as I mentioned, ok. So, there are numerical calculations, people have done and so, those I will not get into, ok.

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To verify $|\Phi\rangle$ is eigenstate of Hamiltonian H , we write Hamiltonian in terms of operators

$$S_i^x = S_i^+ + S_i^- \quad [S_i^x, S_i^y] = -i\hbar S_i^z$$

$$S_i^y = \frac{1}{i}(S_i^+ - S_i^-) \quad [S_i^y, S_i^z] = i\hbar S_i^x$$

$$S_i^z = S_i^+ S_i^- = S_i^- S_i^+ + \hbar S_i^z$$

This Hamiltonian can be written as

$$H = -\frac{1}{2} \sum_{ij} J_{ij} S_i^x S_j^x - \frac{1}{2} \sum_{ij} J_{ij} S_i^y S_j^y - \sum_{ij} J_{ij} S_i^z S_j^z$$

when $S_i = S_i^+ S_i^-$, $S_i^z \geq 0$. It follows that when H acts on $|\Phi\rangle$, only terms in S_i^z contribute to the result. But $|\Phi\rangle$ is constructed to be the eigenstate of each S_i^z with eigenvalue S_i^z , and therefore

$$H|\Phi\rangle = E_0|\Phi\rangle$$

$$E_0 = -\frac{1}{2} \sum_{ij} J_{ij} S_i^z S_j^z$$

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This $|\Phi\rangle$ is indeed an eigenstate of H . To prove E_0 is the energy of the ground state, we consider any other ground state $|\Psi\rangle$ of H with eigenvalue E_Ψ . Since $E_0 \leq \langle \Psi | H | \Psi \rangle$,

it follows that when all the J_{ij} are positive, E_0 has the lower bound

$$-\frac{1}{2} \sum_{ij} J_{ij} \max \langle \hat{S}_i^x \hat{S}_j^x \rangle - \frac{1}{2} \sum_{ij} J_{ij} \max \langle \hat{S}_i^y \hat{S}_j^y \rangle$$

where, $\max \langle X \rangle$ is the largest diagonal matrix element that the operator X can assume.

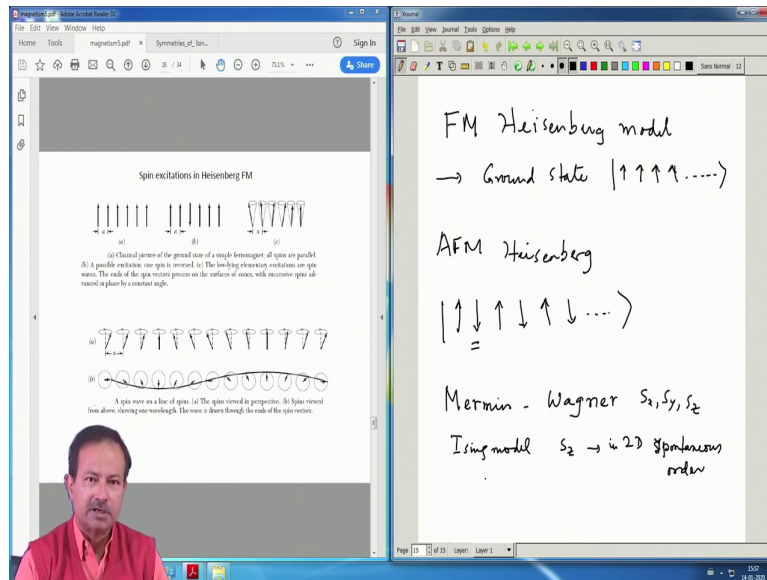
$$\langle \hat{S}_i^x \hat{S}_j^x \rangle \leq S^2 \quad i \neq j$$

$$\langle \hat{S}_i^z \rangle \leq S$$

Combining these inequalities with the bound for E_0 and comparing the resulting inequality with the form of E_0 , we conclude that E_Ψ cannot be less than E_0 and therefore E_0 must be the energy of the ground state.

But those are only approximate, in the sense that is a finite side system where calculations have been done.

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So, the as I said the anti-ferromagnetic Heisenberg model is unsolvable, at least so far we have not been able to solve, no one has been able to solve in any dimension other than one.

The interesting thing about dimensionality which I have been mentioned repeatedly, that dimensionality of the lattice where you are working in the real space dimension, where the spins are or the moments are sitting is actually very important. And of course, the number of components of the spin that you are keeping like in Heisenberg model you have x, y, z, all 3 models, all 3 components are kept that is important. And so, the reason for that is that there are strong theorems, very important theorems that tell us in which dimension with, what kind of spin, how many components of spin you can have a spontaneous magnetization or not.

A famous theorem is that that tells us all this is due to Mermin and Wigner. And this Mermin Wigner theorem tells you that if you have your order parameter which is say magnetization in this case or staggered magnetization for anti-ferromagnets, in either case in dimensions one and two you cannot have ordered state, ordered grounds ordered state at for any order parameter which is continuous.

In the sense that if you have more than one component of the order like for example, if you have spins which have S_x, S_y both components then you cannot have order in any dimension below 2. 6 S_y S_z if you have then of course, you do not have either.

The only case the case where you have order at two-dimension. So, Ising model for example, S_z has only S_z component, no other component exists, in that case in 2D you can have spontaneous magnetization, spontaneous order, ok. But not in 1D, in 1D we showed that at any finite temperature, you do not have any spontaneous order. So, this is basically the content of Mermin Wigner theorem is a bit broader.

But basically essentially for spin models that we are discussing it tells us that for Heisenberg model and models where only x and y components are kept, you cannot have an order spontaneously ordered state at any finite temperature for dimensions less or equal to 2. For Ising model where only you have only one component which is S_z , you can have order in two-dimension, but not in one-dimension spontaneous order.

So, that is this there are comments on this and in many places the book by Ashcroft Mermin, the same Mermin. Also makes a comment, you can go and look up it is a very important theorem and it is to be remembered when you do actual calculations that this thing is this theorem tells us where to look for order and where not to.

The reason for that of course, is again a fluctuations. Now, I will not get into the nature and details of fluctuations, but I will give one example where I will show how thermal fluctuation reduces the value of the total magnetization in a ferromagnetic.

For example, in this Heisenberg ferromagnet that we did, there is a there these fluctuations which can be actually calculated and that fluctuation gives rise to a reduction in the total magnetic moment from its ground state value which is a saturated magnetization saturated value. From that you can which is all spins up. So, that is a saturated magnet magnetic state and which is the ground state for a Heisenberg Ferromagnet. But once you are at any finite temperature of course, this will start fluctuating and the moment saturation value will not be the value of the total magnetic moment. And that is what I will just outline as to why this is important and how this is calculated.

There are many ways to calculate this, very sophisticated methods exist. Here what I do is a method used basically a classical method which works fairly well, but it is it gives the result which I want to show you.

So, spin excitations in the Heisenberg ferromagnet, ok. So, what are the excited states? So, when the temperature is finite of course, the ground state will have excursions into the spins will start fluctuating and there will be excursions into the higher energy states, and that is what thermodynamics is all about and so this description basically tells you how to calculate the energies of such states, what are these excitations and so on..

So, in a ferromagnet for example, a pictorial representation is like this, that the spins are start starting to rotate. So, if they were totally up, so spins were up originally and now they start to rotate about it. And since the tilt and rotate the magnitude starts decreasing from the saturation value and so, the net value will be net magnetisation will decrease from the saturation value.

So, these pictures actually show value from this. The way these fluctuations take place from the side view and the spins from the top view you can see that the spins are rotating. And they are rotating we take a particular wave vector wave length λ . So, this wave length can be very large and the larger the wave length and the lesser is the cost again such excitations.

Every excitation costs energy. So, it is it can be shown that as this wave length becomes larger and larger, the angle between nearest neighbour spins is very small then, exceedingly small and as the wave length becomes very large. And therefore, the even classically if you think of the energy as $S_1 \cdot S_2 \cos \theta$ between two spins, then if θ is exceedingly small of course, your energy goes as θ^2 and you can expand $\cos \theta$ and get θ^2 term and that is very very small if θ is small.

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Magnons

- A magnon is a quantized spin wave.

The ground state of a simple ferromagnet has all spins parallel. Consider N spins each of magnitude S on a line or a ring, with nearest-neighbor spins coupled by the Heisenberg interaction:

$$U = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_{j+1}$$

(a) Classical picture of the ground state of a simple ferromagnet: all spins are parallel. (b) A possible excitation: one spin is reversed. (c) The low-lying elementary excitations are spin waves: the spin vectors precess on the surface of cones, with successive spins at constant angle.

So, these excitations when they are quantized are called Magnons. Now, a magnon is basically a quantized spin wave. So, this kind of wave structure of spin is called a spin wave, and this when you quantize are called magnons. So, let us just try to calculate from this Heisenberg Hamiltonian. So, it is a classic calculation goes classically ah. So, let us just go one more step, ok.

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Diagrams illustrating spin waves on a line of spins. (a) The spin vectors in a propagating spin wave are shown precessing around the z-axis, showing wave motion. The wave is shown through the ends of the spin vectors. (b) The wave is shown through the ends of the spin vectors.

Handwritten equations on the right:

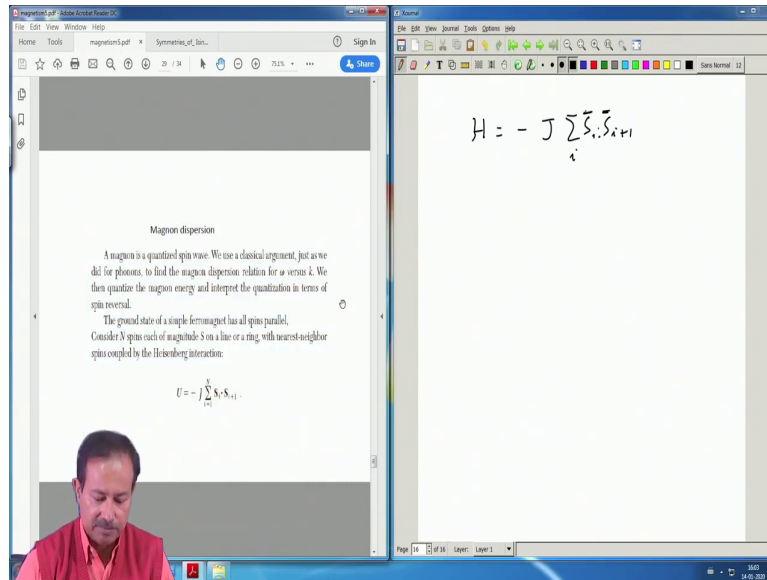
$$H = -J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}$$

$$\frac{dS_{iz}}{dt} = S_{iz} = S$$

$$\frac{dS_{iz}}{dt} = (S_x, S_y) = S_x S_y$$

This again shows in a coloured picture as to how this spins are rotating about their original around the magnetic field for example, which is the original direction of the magnetization. And this is the wave length for example, ok. Excuse me.

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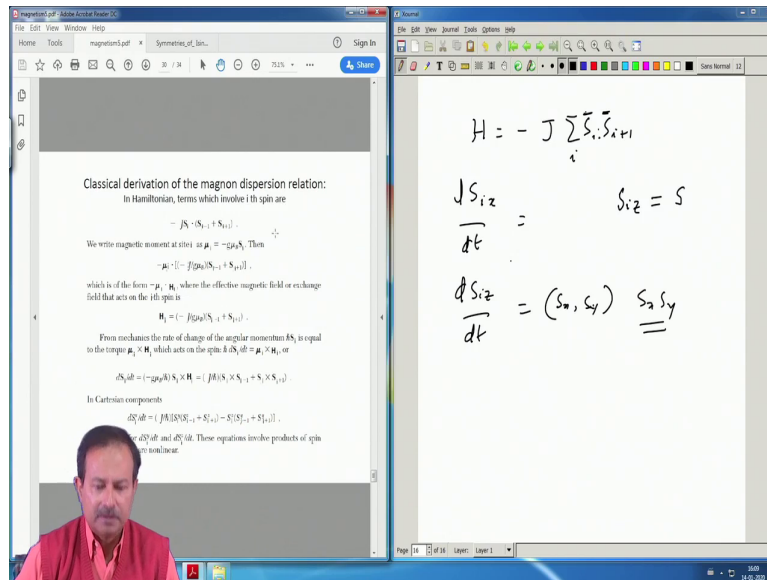


So, let us just start calculate the calculating the ground state of a simple ferromagnet has all spins parallel and then consider n such spins magnitude S on a line. So, let us do it for a one-dimension, for example on a line.

So, and then you can rotate the put periodic boundary condition took make it into a ring and the Hamiltonian here is only nearest neighbour. So, the Hamiltonian as you as we wrote down earlier for one-dimension is minus $J S_i \cdot S_{i+1}$ all higher neighbour interactions are 0. So, and then between i and $i + 1$ the interaction is J .

So, that is the simplest model, the nearest neighbour Heisenberg model in one-dimension with ferromagnetism. That is what is being written down. These are vectors and so, that is the model where we are going to study and try to find out its excitation spectrum, ok.

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So, the classical derivation goes like this. Take for example, the i th spin, so i th spin interacts with i minus 1 and i plus 1 on two sites. So that means, I can think of like in mean field theory I can think of the i th spin being acted on by a magnetic field that is coming from these two moments, these two spins, i plus 1 and i minus 1. So, that is the moment that is the magnetic field that is we written here this H equal to i minus coming from i plus 1 and i minus 1 spins.

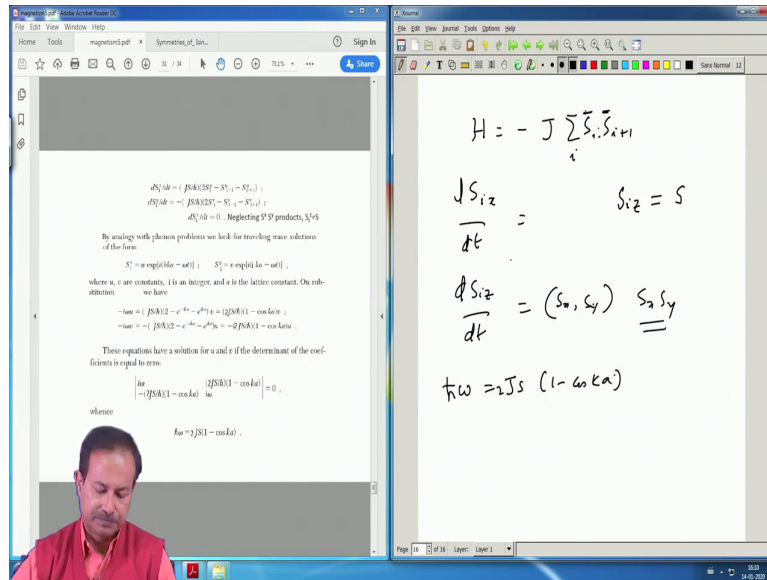
And this is what we will use now and we will just write the classical equation of motion which is basically the force; angular momentum is change due to the torque μ cross H and that H is this. So, the i th moment has a torque on it due to the magnetic field coming from the two neighbouring spins, ok. So, that is equation is this, ΔS_i is. So, for example, for the i th spin it is i minus 1 and i plus 1 with S_i crossed with S_i . So, that is the classical equation of motion.

In Cartesian, divide it into Cartesian components. So, write the equation of motion for dS_x / dt equal to sum this, this is the result right, it involves y and z components because it is a cross product. So, this that is all you have, ok. Similarly, you can write for S_y and S_z .

Now, the assumption here is that that these deviations from the z axis the deviations, see no in the ground state there was no x and y components all z only. Once you start deviating you

generate x and y components. Now, if these deviations are exceedingly small then the x and y components are very very small. So, we will neglect all S x square, S y square, their squares, ok, so that is what is the assumption here is.

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So, under that assumption you can write down the equation of motion which is these two will have, see the S x has y and linear in y, and then the S z is z is replaced by S. It is fully saturated value because the deviation from S is very small as I said. So, at each site and each spin, so this is replaced by S, and S x and S y are kept.

But what is not kept is on the right hand side of S z the equation for S z d S i z dt, you had only x and y component, S x and S y components right and their products. So, the product is of order S square, S x square or S y square or a combination of S x and S y and it is actually a combination of S x s. So, it is always like S x, S y. So, these combinations are neglected because both S x and S y are considered to be very very small. So, there the quadratic terms are neglected. So, that is why the right hand side here is 0, ok.

So, that is what I is written here S x S y product are a set to 0 and S z is taken to be S. Then of course, you can draw analogy with the phonon problem for example, which is a very similar problem where each phonon each site is coupled to the two nearest neighbours on its

sides for vibrations. Remember your coupled oscillator. So, one oscillates the other one comes closer and so on and so forth. So, this is a very similar problem.

There the coupling constant was k , potential was Kx^2 . Here the interaction is $J S_i S_{i+1}$. So, that is that that is that is the difference of course. Of course, these are two different problems. So, the analogy only is in this the kind of equations you get they are, so S_x at i site is coupled to it is too nearest neighbours. So, is why at i site is also coupled to its nearest neighbours and then of course, one can look for a traveling wave solution of these kind. And this solution is this and the other one similarly for the other one.

Now, put it back in. See this is a general principle of translational invariance because there is no site is unique in a Hamiltonian which is translationally symmetric and that is being used here also. So, once you deviate a spin that deviation does not stay there, I mean that deviation moves and that is these pictures actually tell you that that the deviation is not localized, the deviation basically moves and it this spin rotates. So, ever it goes to all the states. So, any deviation will we will pass through this trough and the crest will pass through every spin.

So, that is like a traveling wave. And that is because there is a translational symmetry. There is no spin which is a single down, where you will only have the trough or the minimum. So, that is, so that is being used here and that gives us gives us this these kind of equations. And it is a 2 by 2 matrix equation in terms of u and v , and you know how to solve such equations. All you have to do is to just diagonalize that matrix that will give you the energy the corresponding to this modes u and v , ok. We did modes that u and v combined to give you.

So, there are these, this is the energy and energy for the traveling wave which is called the spin wave and so this if you quantize will give you the magnons, ok. So, this is a this is an energies which is very simple $\hbar \omega = 2JS(1 - \cos Ka)$.

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So, Ka inverse of K , K is basically 2π by λ , so it tells you what is the wave length is. Smaller the K the larger the wave length and so that means, the less is the cost of the excitation. And this indeed is the case. You can expand the $\cos K$ for Ka much less than 1, Ka much much less than 1 you can expand. And $1 - \cos K$ is then half K half Ka square. And this means that the energy is quadratic in K . This is different from phonons though. So, that is why I did not want to draw the analogy too far because this is not really the same calculation that we are doing. In phonons this is linear in K .

So, here it is like a free like a free particle. Actually, it is a K square spectrum which is like a p square by twice m that we do. So, to 1 by twice m will be this $2JS$ half, so this JS basically. So, that is what it says that in the same limit the frequency of a phonon is proportional to K , not K square. So, this spectrum is therefore, like this, and a K square spectrum is generally termed as a free particle spectrum.

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Thermal Excitation of Magnons

In thermal equilibrium the average value of the number of magnons excited in the mode k is given by the Planck distribution

$$\langle n_k \rangle = \frac{1}{\exp(\hbar\omega_k/kT) - 1}$$

The total number of magnons excited at a temperature T is

$$\sum_k n_k = \int d\omega D(\omega) \langle n(\omega) \rangle$$

Magnons have a single polarization for each value of k . In three dimensions the number of modes of wavevector less than k is $(1/2\pi)^3 (4\pi k^3/3)$ per unit volume, whence the number of magnons $E(\omega)/d\omega$ with frequency in $d\omega$ at ω is $(1/2\pi)^3 (4\pi k^2) dk/d\omega$

$$\frac{dE}{d\omega} = \frac{2N\hbar\omega}{k} = \left(\frac{2N\hbar^2}{k}\right) \omega^2$$

Whiteboard notes:

$$H = -J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}$$

$$\frac{dS_{iz}}{dt} = S_{iz} = S$$

$$\frac{dS_{iz}}{dt} = (S_x, S_y) = S_x S_y$$

$$\hbar\omega = 2JS(1 - \cos ka) \sim \frac{1}{2}(ka)^2$$

$ka \ll 1$ $\omega \sim k^2$

(A small graph showing a parabolic curve is drawn below the boxed equation.)

Now, once I have these spectrum this energy then I can calculate in thermal equilibrium how many magnons are there at a particular temperature. So, that is basically these magnons are bosons. If you quantize you can see that they are bosons and these the number is given by the Bose statistics. And the total number can therefore be calculated by the same principle that we used the density of states of these phonons. See that these phonons have a k square spectrum. So, they will also have a root over energy kind of a density of states as similar to what we got for free particle.

So, that is $d\omega$ here, a times this $n\omega$ and here is the $d\omega$ being calculated, so then what you get is $d\omega$ is proportional to ω to the power half, ok.

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So, here of course, what you have is you want to calculate this n of k, the total deviation from the from the number of. So, we were basically calculating the number of magnons. So, that will basically tell you how much you have deviated from your saturation magnetization. So, that number itself is the deviation from the saturation magnetization. So, that is what one is trying to calculate and so, let us just see what you get.

See this is n k somewhere all k and that is this integral becomes like this. You can convert into a dimensional dimensionless integral which is often done and the integration can be taken from 0 to infinity because the density of states vanishes then the energies the there are no phonons at infinity and had no magnons at infinity energies and so on and so, forth. So, all that is taken care of. You can take these limits from 0 to infinity.

So, then what you find is this kind of a of an integral where this if you look at this last piece inside the integral it is inside, it is dimensionless integration, everything here is dimensionless. So, this is just a number. The all the temperature dependence is outside. And this is what you do in phonon in the device specific it calculation as well, then what you find is that there is a temperature dependence which is T to the power 3 by 2. This temperature dependence 3 by 2 was obtained first by Felix Bloch, the person in whose name Bloch theorem is.

And he showed that there is a deviation from the saturation magnetization at finite temperature. And this number itself is the Δm , the change in m from the finite value, from the saturation value and that number if you calculate that integral you can find this numerical values are obtainable and one finds $k_B T$ by $J S$ to the power $3/2$.

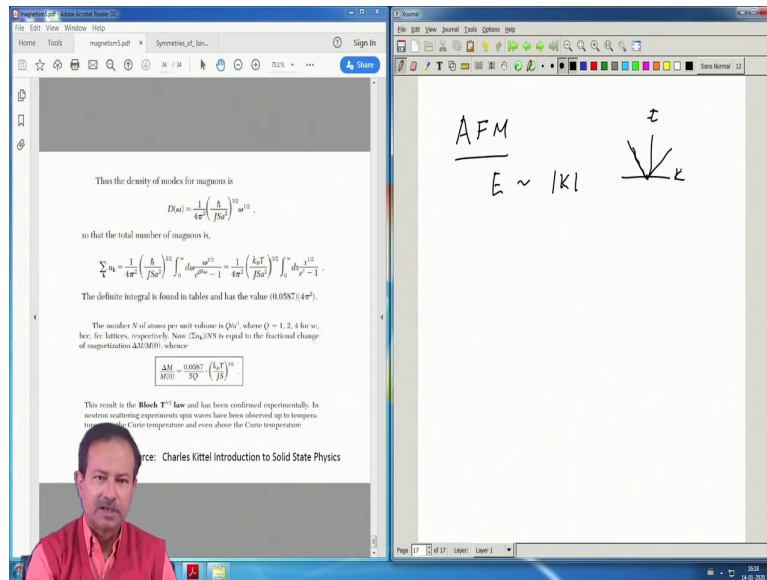
So, this is the see ΔM by M , ok. So, this is a dimensionless quantity on the left should have a dimensionless quantity on the right, but the power of temperature is T to the power $3/2$. So, this is called Bloch's T to the power $3/2$ law and it is confirmed experimentally.

This is how the magnetization deviates at finite temperature in a ferromagnet and this is obtained by neutron scattering, ok. And this is this treatment you will find in charge skittles book, solid state physics and in many other places, but there are as I said much more sophisticated techniques available where you start by writing down the bosons and then see the spin flip is like a boson.

For example, take spin half. You are going from plus up to minus up or minus up to plus up you are changing the spin by 1. So, these flip if you can quantize the flip you will see there is a spin is a even spin object. So, that is it changes the spin by 1 basically and that is even and that is that will follow both statistics.

The case for anti-ferromagnet is much more complicated. For AFM first of all we do not know the ground state except in one-dimension, where it is not a state of that kind that I wrote up down, up down, up down that is generally called a Neel state.

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Now, that is not even an eigenstate. So, let us forget about it. But the spin of calculation is still done with respect to the classical ground state which is the anti-ferromagnetic state and one can calculate, then in that case one can calculate and one finds that its more complicated calculation the energy or the omega that we wrote here in this case will go as mod of K, instead of K square. So, it is a steeper. So, it is much more steep. It is like this. And that is a E versus K for AFM, and that has profound consequences.

And the only thing I would mention is that that we are calculating fluctuations, but these are all thermal fluctuations There are things called quantum fluctuations which are important and for an anti-ferromagnet for example, that already reduces the magnetization from the, from its saturated value. And so, those are beyond the purview of this course, but it is those who are interested can look up the literature and find out the case for antiferromagnet which is a really interesting situation and if you are really interested you can look up. But as I said that there is already in ferromagnet there are these magnons at finite temperature which will reduce the magnetization from its saturation value.