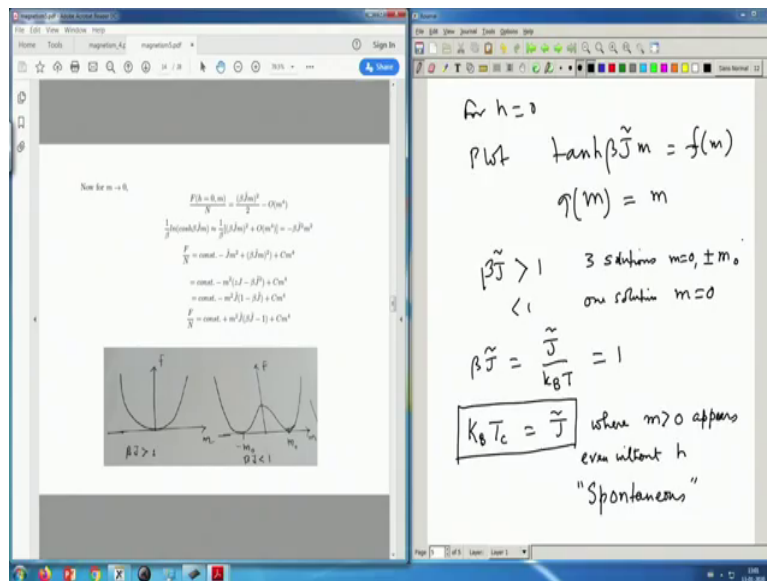


Electronic Theory of Solids
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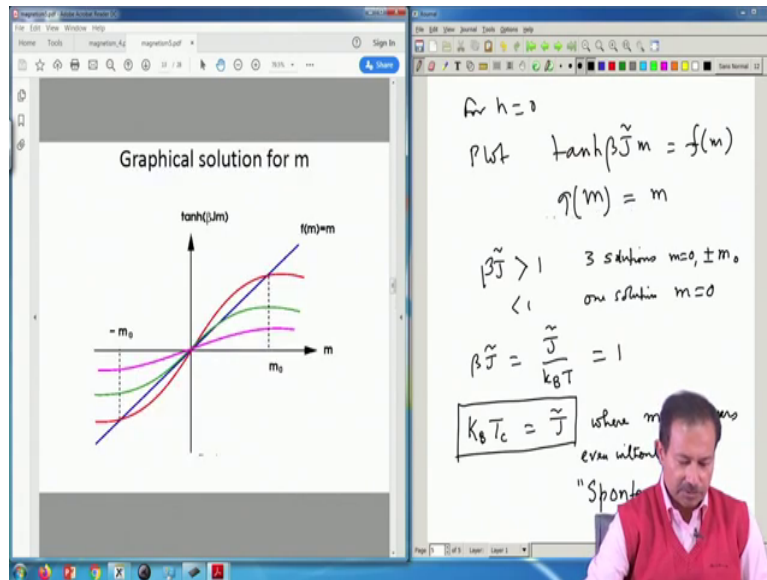
Lecture - 43
Spontaneous magnetisation & 1D Ising Model

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So, we have been doing a Ising model in the mean field theory. And, in mean field theory what we found out is that the, there is a finite temperature at which the system becomes a say ordered magnet, all spins in one direction with a finite magnetic moment m sub 0.

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So, that is what we showed here depending on whether you have above this value of T_c or below. If you are above then you have a solution only m equal to 0. If you are below it then you start picking up solution and as you come down in temperature, the intercept becomes happens at a larger and larger distance and at very low temperature as you can see this intercept will not change much because tan hyperbolic will saturate.

So, then, you are basically at a fully saturated ferromagnetic state where all spins are completely up ok. So, at 0 temperature of course, every spin will give you plus 1. So, the total moment will be just n all spins up ok.

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So, this analysis can be taken a bit further which is actually very relevant, because there is a famous theory by Ginzberg and Landau where they expanded the free energy close to T_c in terms of something called an order parameter. An order parameter is something which is 0 below T_c which is non-zero below T_c and 0 above T_c . So, that is like magnetization here, magnetization is above T_c 0, magnetization below T_c is non-zero. So, this is a quantity by which you can distinguish between the spontaneously ordered state and the disordered state which is like a paramagnet.

Now, so, they what they did was that they wrote down the free energy in an approximate manner, just wrote down as a polynomial in this order parameter and their derivatives that are allowed by the symmetry. Nevertheless I we will not do that, but we will do something analogous to it which is that what we will do now is to adjust expand free energy that we got from the mean field theory to second order to fourth to order fourth order in the magnetization and this is what you will get.

So, what you will get is F by N . So, free energy density for example, per part spin is some constant plus this $m^2 J \tilde{\text{into}} \beta J \tilde{\text{minus}} 1$ plus $C m^4$. Now, if you look at your graph of this quantity on the right hand side constant you can just absorb and set it to 0, absorb inside the energies. So, what you have is F versus m plot in two situations.

Where βJ is greater than 1; so, the coefficient of this m^2 term is positive. So, coefficient of m^2 positive, greater than 0. In that case you get this first curve which is like a parabola and then of course, this m^4 term, which will make it much steeper than a parabola. And, then there is only one minimum of this you want to minimize the free energy that is the solution. So, $m = 0$ is the only solution, so that means; $m = 0$ which means that it is a disordered state you are actually above your T_c .

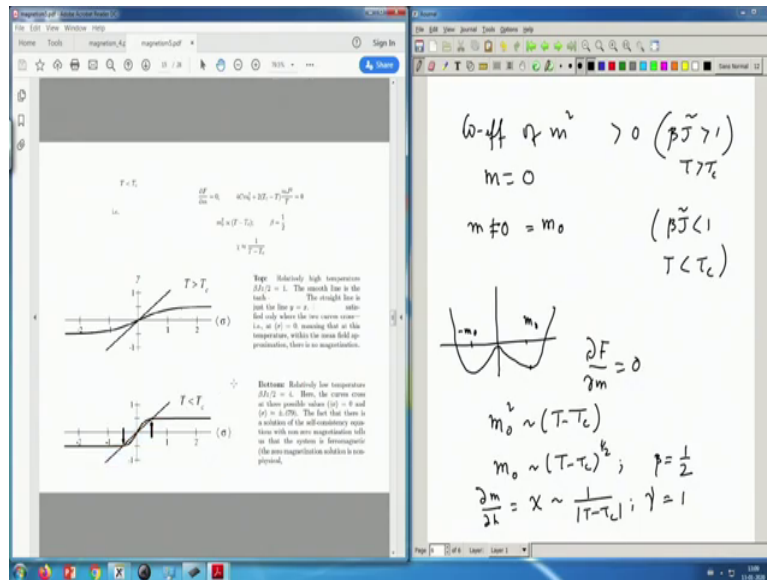
So, that is βJ greater than 1. Now in the other case where βJ less than 1, that is see J is $1/k_B T_c$; so, $T < T_c$. So, this is $T > T_c$. So, in that case you will land up with a curve which is like this, the free energy looks like this with the minimum at $m = 0$ has now become a maximum, local maximum. And that the, the at minima where the minimum has now gone into two sides, which is symmetric; this curve is symmetric remember it is an even function.

So, $m = 0$ and $m \neq 0$ at the two minima now. So, that means, you have a situation where you can have if I absorb the constant into 0, then I will have this kind of a situation, $m = 0$ and $m \neq 0$. So, then, you have just these two minima these are the solutions. So, in that case $m \neq 0$ and the system is spontaneously magnetized.

So, just by expanding the free energy and looking at the coefficient of the quadratic term in the order parameter, this is m here is the order parameter which is non-zero below T_c and 0 above T_c . One can actually tell whether the system is spontaneously ordered or not. And, at the point where this ordering takes place where the coefficient goes from positive to negative you will have an order and that is where the T_c is, that is how T_c is formed in this kind of a theory.

This is a very celebrated theory by Ginsberg and Landau which was which has actually helped understand phase transition and critical phenomena enormously.

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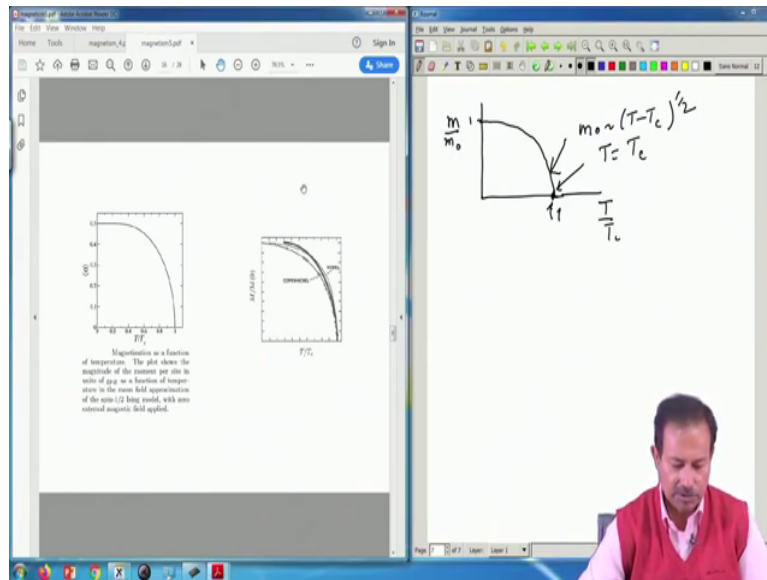


So, this is again the same thing, from that one can actually do more if you set $\frac{\partial F}{\partial m}$ equal to 0 $\frac{\partial F}{\partial h}$ equal to 0, you can find out the value of m naught. And you can see that m naught square is proportional to T minus T_c , it is just one line calculation, I leave it for you to do. And, that means; m naught goes as T minus T_c to the power half, this exponent half in mean field theory is always half and this is called the beta exponent, this exponent is half in mean field theory.

Similarly you can keep the magnetic field do the expansion and calculate $\frac{\partial m}{\partial h}$ which gives you χ and that there you will find that χ goes as 1 by T minus T_c . And that is, that means; this exponent that means, χ goes as T minus T_c to the power minus 1 , so that exponent is called gamma, that gamma exponent is 1 . So, these exponents are actually measured experimentally close to T_c , this is how they behave. And in mean field theory, you can actually find out the coefficient with these exponents and these exponents are beta equal to half and gamma equal to 1 .

This picture on the left actually shows you how greater than T_c how it behaves, less than T_c how it behaves from a mean field theory you can work it out.

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And then of course, you can work out the entire graph and this is remarkable because, this is the graph for order parameter m the magnetization here versus T by T_c . And, at T by T_c is equal to 1 you will see the and this say this m by m naught at 0 temperature this is full m naught, so this will be 1 and then slowly it will come down and it will come down very rapidly close to the 0.1, so this is the 0.1 ok.

So, this is 1, that is T equal to T_c . So, this is how it happens and the here if you find out m naught as a function of T you will see that it will be T minus T_c to the power half which is again that that exponent half close to T_c this is how it behaves. And, this is a graph you will see in many many places in phase transition, how m goes as varies with T . And typically, in many places you will find this T minus T_c to the power half behavior and its sort of universal in certain class of systems with I mean there are caveats, but in mean field theory it is always t minus T_c to the power half.

So, if you find a curve for an order parameter behaving like this, then you can realize that this is like a mean field transition, mean field phase transition that is happening so, so far so good.

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Exact solution in 1D

Partition function:

$$Z = \sum_{s_1=-1}^{+1} \sum_{s_2=-1}^{+1} \dots \sum_{s_N=-1}^{+1} e^{-\beta E(S)}$$

PBC: $s_{N+1} = s_1$

$$E(S) = -J \sum_{i=1}^N S_i S_{i+1} - H \sum_{i=1}^N S_i$$

Transfer Matrix (Kramers and Wannier 1941)

$$Z = \sum_{s_1=-1}^{+1} \dots \sum_{s_N=-1}^{+1} \exp \left[\beta \sum_{i=1}^N \left(JS_i S_{i+1} + \frac{1}{2} H(S_i + S_{i+1}) \right) \right]$$

Define 2x2 matrix: $(S_i P_j S'_i) = \exp \left\{ \beta \left[JS_i S'_i + \frac{1}{2} H(S_i + S'_i) \right] \right\}$

$$\begin{aligned} (+1|P|+1) &= \exp[\beta(J+H)] \\ (-1|P|+1) &= \exp[\beta(J-H)] \\ (+1|P|-1) &= (-1|P|-1) = \exp[-\beta J] \end{aligned}$$

Mean-field: finite $T=T_c$ where spontaneous magnetisation occurs

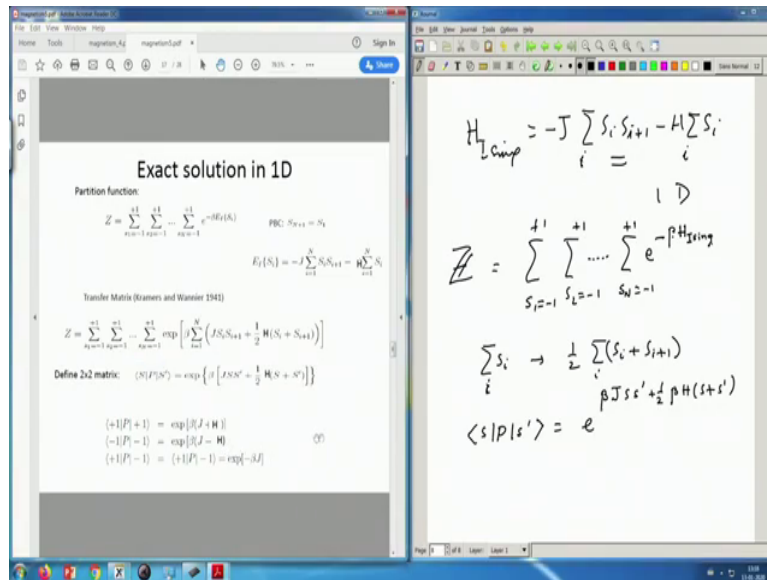
$\beta = \frac{1}{2}, \gamma = 1. \chi \sim (T-T_c)^{-1}$

Now, I want to show you something which is a very simple calculation, but this is one of the rare cases where one can solve a model a spin model exactly. And, that is just for showing you do not have to remember the calculations neither do you have to find out the have to repeat and cram all these things.

Just look at the calculations it is simple, it is doable and it is a rare opportunity to do an exact solution and that is that also reveals something remarkably interesting. So, let us just summarize what we found from mean field theory. So, mean field results are mainly this; there is a finite T equal to T c where spontaneous magnetization occurs, right. So, T c is finite, where magnetic moments are finite, total moment is finite.

And the other thing is that these exponent beta of half and gamma equal to half gamma equal to 1. So, gamma means susceptibility goes as T minus T c to the power minus gamma, that exponent gamma is 1. Now, what I do is to solve this model in one dimension exactly and show what happens, to contrast it with the solution that I obtain from the mean field theory.

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Again I am repeating that you do not have to do this calculation if you like you can do it, but it is just a very simple calculation beautiful calculation and let me show you how it is done. So, again you go back to the model with a field and field is written as H here this is the field. So, the model is $J S_i \cdot S_{i+1} + H \sum_i S_i$. Since it is one dimensional as I said I can write it as $S_i S_{i+1}$, no bond is now double counted.

Now, the and is the magnetic field ok. So, partition function as we all know how to calculate is basically all possible configurations you have to sum over them and, so this is S_1 from minus 1 to plus 1, minus 1 and plus 1, there is no continuous summation, just minus 1 and plus 1. S_2 , similarly minus 1 plus 1 and so on.

S_N minus 1 to plus 1 e to the power minus beta this beta times this H, which is written here as $e^{-\beta H}$ this curly bracket means all configurations of S_i so, all the S_i . So, S_i is $\sum_i S_i$ is written here ok. So, beta I can also write this beta H Ising, minus beta H Ising. This board is not very comfortable, but let me just try to make it simple write it again.

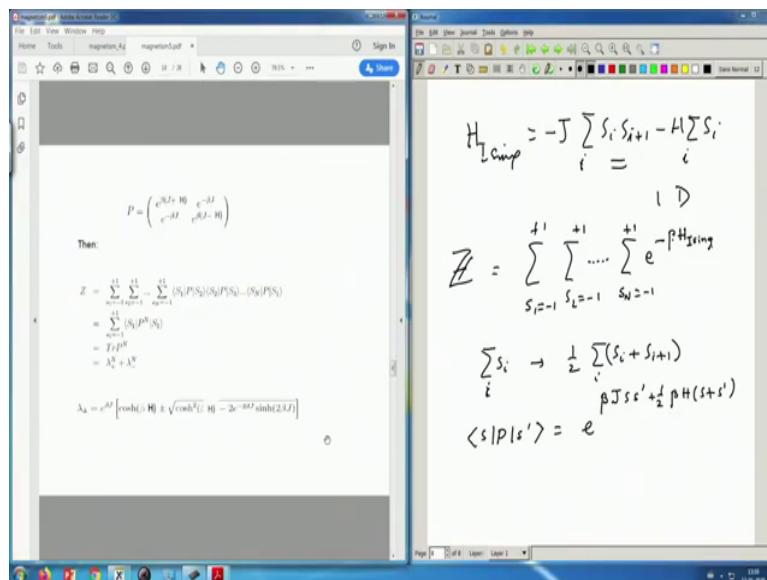
So, now, this is this is what you are doing. Then you can recast this partition function as is done here. All you have done is that you have written this H, the summation over H, summation over S_i , you have represented by half $S_i + S_{i+1}$, which means every spin is now summed twice, but i and $i+1$ are put together. So, that is why the half comes ok.

So, that is exactly what has been done in this, this line in this line ok. Now is the trick this trick is was first done by Cramers and Wannier, two of the greatest physicists of the last century and these trick implies that you write a 2 by 2 matrix defined by this, this is written here. This is the matrix S between S and S prime, so, the matrix elements of S and S prime, S and S prime will take values plus 1 minus 1 both right like a size S P S prime.

And, it is written as e to the power beta J see the Hamiltonian had a minus that is why you get a plus here e to the power beta J S S prime plus half beta H S plus S prime. So, that is what this so, this is an operator you have to take S and S prime on both sides and find out the matrix element four the four matrix elements. So, these four are plus 1 when S and S prime are both plus 1 they are minus 1 and one is plus 1 and the other one is minus 1 and this is symmetric S P 1 P 1 2 is equal to P 2 1, P 1 2 is this, P 2 1 is this.

So, that matrix you can easily calculate S and S prime both for example, both positive J S S prime. So, it is beta J and then both of them are plus 1, so 1 plus 1 divided by 2 is just H; so, J plus H similarly for the others.

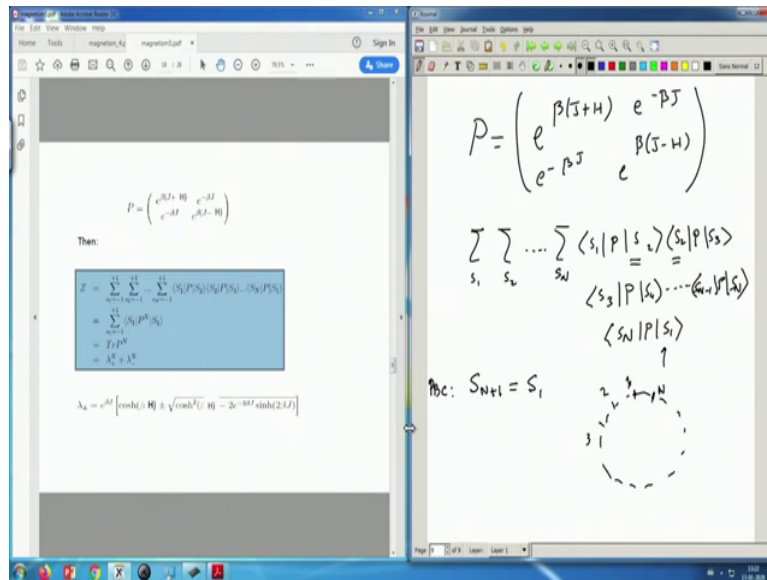
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So, that is the for example, this one, plus 1 and minus 1, so this will be plus this will have plus 1 minus 1 means minus J, this one, but the second term will vanish because, there will be no H because this is plus 1 and this is minus 1 and similarly, when S prime is minus 1 S S is

plus 1, this will also vanish. So, there will be no H in the off diagonal terms which is just into the minus beta J.

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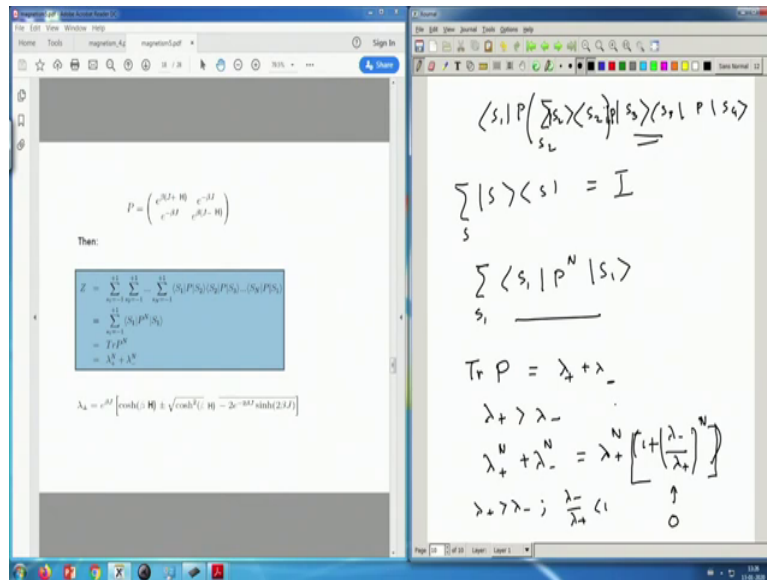


So, the matrix then looks like simple it is just a 2 by 2 matrix, P equal to e to the power beta J plus H, e to the power beta J minus H, e to the power minus beta J, e to the power minus beta J is a symmetric matrix. Now, you can just look at how you can recast the summation in the partition function on the right hand side, this is really interesting.

So, you can check for yourself you can actually do it and check it for yourself that you just put this matrix here and you will see that this summation on the right S_1, S_2, S_N is basically $S_1 P S_2, S_2 P S_3, S_3 P S_4$, so on, S_N minus 1 $P S_N$ ok and then S_N and then $S_N P S_1$. Now, this last one comes from the periodic boundary condition where we have identified S_N plus 1 equal to S_1 . So, it is now the spins are like on a ring.

So, this is the first spin, this is the Nth spin, so this is N this is 1, 2, 3 and so on and the N plus 1 is the same as N. So, this is like a ring now the topology is a ring. This is the periodic boundary condition that we used in Born Von Karman boundary condition as well. So, this is just that periodic boundary condition put in here. So, this is PBC. Now the interesting thing to note is that there are this sum for example, sum over S_2 where does S_2 appear S_2 appears only here and here.

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So, I can actually take this S 2 sum somewhere here which is what I let me just do. So, I have S 1 P then I do this S 2 sum. So, let me just do it, let me S 2 then S 3 right, P S 3, P S 3, P S 3. Now, look at this, this is just a ket and bra. So, this kind of things student, S sum over S basically, identity from quantum mechanics.

So, that means; I can actually do it for every of these, I will I can also do for S 3 which has an S 3 here, then P, then S four right. So, for these also I can take this S 3 sum inside and sum over this and get identity. So, all of these will become identity except for the first one at the last one and what are those you will be left with only S 1 S 1 P to the power N S 1 right and that, is exactly what is shown here.

So, this summation basically reduces to a trace calculation of the matrix P to the power N of course, that is also nontrivial because this is a 2 by 2 matrix you have to multiply it by N times. And, find out find that out and if N is very large which is true N is thermodynamically large number often take into infinity, then it is this is also not simple.

But, what is simple is that we know the trace is invariant under similarity transformation and so, what we will do is that we simply diagonalize this matrix P. And, then the trace of P, trace of any matrix is basically the sum over the diagonals. Suppose you diagonalize this matrix,

then trace of P is just the sum over the diagonals and the trace is invariant, this is also this is a trace.

So, all I need to know is λ_1 and λ_2 , the two eigenvalues of this and that they are they are written here as λ_+ and λ_- . So, let me also do it λ_+ and λ_- . So, these are the two eigenvalues I need to know that is all. So, the entire problem has reduced to finding out these two eigenvalues, which is a 2 by 2 matrix, I can find the eigenvalues and this is what the eigenvalues are.

And now suppose, λ_+ is greater than λ_- , then λ_+ to the power N plus λ_- to the power N is I can take λ_+ common to the power N common, then $1 + \lambda_-^2$ the power N divide by λ_+ to the power N . Now, this quantity, so this let me just put a bracket here, let me put a bracket here. This is the quantity I have to calculate, right.

Now since λ_+ is greater than λ_- λ_- divided by λ_+ less than 1 and if N is very large, this quantity actually goes to 0. It is exceedingly small, if say N is millions, zillions or trillions or whatever 10 to the power 23 is a typical number in a real system, then any quantity which is less than 1, if you multiply it by even by 10 times it will become almost 0. So, you can actually neglect this term without any problem. So, all you are left with is just λ_+ to the power N and that is all you do.

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Helmholtz free energy per spin:

$$\begin{aligned} \frac{F}{Nk_B T} &= \lim_{N \rightarrow \infty} \frac{1}{N} \ln Z \\ &= \lim_{N \rightarrow \infty} \frac{1}{N} \ln \left\{ z^N \left[1 + \left(\frac{z}{\lambda} \right)^N \right] \right\} \\ &= \ln z + \lim_{N \rightarrow \infty} \frac{1}{N} \ln \left[1 + \left(\frac{z}{\lambda} \right)^N \right] \\ &= \ln z, \end{aligned}$$

So the Helmholtz free energy per spin is

$$\begin{aligned} \frac{F}{N} &= \frac{k_B T}{N} \ln Z = -k_B T \ln z, \\ &= -J - k_B T \ln \left[\cosh(\beta J) + \sqrt{\cosh^2(\beta J) - 2^{-2\beta J} \sinh(2\beta J)} \right]. \end{aligned}$$

$\frac{F}{N} = -k_B T \ln Z$

So, these are the two eigenvalues out of which you will only keep one and so, so this will become so called is. So, here straight here it is straight away one calculates the free energy is minus K B T log of Z and in evaluating Z, you will keep only that lambda plus. So, only Z for lambda plus is required and that is what is done here. So, the F that you get is what is written in the bottom. From here you can now calculate m which is the magnetization.

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The magnetization per spin is

$$\begin{aligned} m &= \frac{M}{N} \\ &= \frac{1}{N} \frac{\partial \ln Z}{\partial \ln z} \\ &= \frac{1}{N} \frac{\partial \ln Z}{\partial \ln z} \\ &= \frac{\sinh(\beta H)}{\sqrt{\cosh^2(\beta H) - 2^{-2\beta J} \sinh(2\beta J)}} \end{aligned}$$

At zero field ($H=0$), the magnetization is zero for all temperatures.

$\frac{F}{N} = -k_B T \ln Z$

$$m = \frac{\sinh(\beta H)}{\sqrt{\cosh^2(\beta H) - 2e^{-2\beta J} \sinh(2\beta J)}}$$

$H \rightarrow 0 \quad m \rightarrow 0$

$F = U - TS$

And, that is this value this formula due to. So, m is \sin hyperbolic βH external magnetic field divided by this denominator \cos hyperbolic square βH minus 2ϵ to the power minus $2\beta J$, \sin hyperbolic $2\beta J$ just look at what happens as H goes to 0 at 0 field external field is 0.

As external field goes to 0, \sin hyperbolic term goes to 0. This goes to 1, this goes to 0. So, you have m going to 0. So, now look at the result it is very different from what we got from the mean field theory. So, in mean field theory at a particular temperature, at any finite temperature which is where we are now β is taken to be finite so T is finite here, so that means; m goes to 0 at any finite temperature as long as h goes to 0.

So, there is no spontaneous magnetization at any finite temperature, that is what this says. Remember as β goes to infinity of course, then this will not work and that is exactly what happens at T equal to 0. At T equal to 0, only at T equal to 0 you will find there is a finite magnetization.

At any other T you can see that, so this is βJ equal to nonzero, the dashed curve is for any βJ non-zero and the this curve is for βJ equal to when T goes to 0, this is this straight line. So, this will become a vertical straight line at β equal to 0. So, so this will just become a vertical line at β at β equal to infinity at any finite temperature it will be like this.

So, this will be m versus h . So, this is T equal to 0 and this is T greater than 0. As of course, as field if field is finite of course, then you will have a finite magnetization that is true, because field will align, but when we discuss spontaneous magnetization we mean that without the absence of field ok.

So, and that is a result that we get here which is dramatically different from the result which is at in the mean field theory. So, the mean field theory is not correct here, it does not give us the right result. The reason for that is that in low dimensions entropy the fluctuation due to temperature leads to an entropy.

So, F is U minus TS remember and only at T equal to 0, entropy contribution is 0. I mean you do not have any entropy contribution whereas, at any finite temperature; the free energy has

an entropy contribution and it is true that at one dimension of Ising in Ising model the entropy contribution always wins at any finite temperature and makes the system disordered and you have no chance of having an ordered state spontaneously ordered state.

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Thermal properties

main thermodynamic quantities are then

$$F = -T \ln Z = -T \ln 2 - NT \ln 2 \cosh(J/T)$$

$$U = \frac{\partial}{\partial \beta} \ln Z = -NJ \tanh(J/T)$$

$$C = \frac{\partial U}{\partial T} = N \left(\frac{J}{T}\right)^2 \operatorname{sech}^2(J/T)$$

$$S = \frac{U-F}{T} = \ln 2 + N \left(-\frac{J}{T} \tanh(J/T) + \ln 2 \cosh(J/T)\right)$$

$$\frac{F}{N} = -k_B T \ln Z$$

$$m = \frac{\sinh \beta H}{\sqrt{\cosh^2(\beta H) - 2e^{-2\beta J} \sinh(2\beta J)}}$$

$H \rightarrow 0 \quad m \rightarrow 0$

$F = U - TS$

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Thermodynamic quantities for the Ising model under zero field

$\frac{F}{N} = -k_B T \ln Z$ $\rightarrow H$
 $\rightarrow -H$

$$m = \frac{\sinh \beta H}{\sqrt{\cosh^2(\beta H) - 2e^{-2\beta J} \sinh(2\beta J)}}$$

$H \rightarrow 0 \quad m \rightarrow 0$

$F = U - TS$

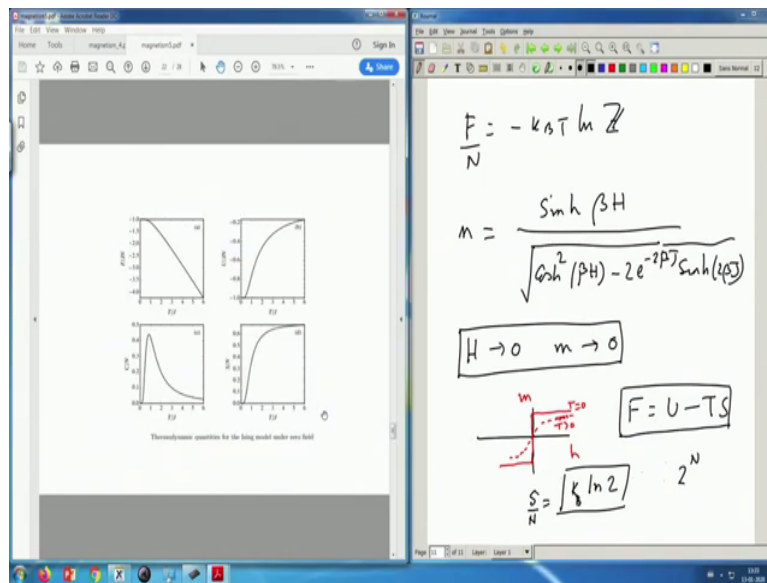
And, that is exactly what the exact result tells us that. And so these are some results the you can calculate free energy, internal energy, specific heat, entropy, everything because these are all exact results this is how it remember this specific heat curve which is again looking like a

Schottky anomaly. Because, you have a state with two levels plus plus see there is this plus H times S.

So, plus H and G mu B plus h and minus H for spin up and spin down, a two level system; so, again at some scale of temperature there will be a peak. So, that is what is happening and then of course, its it falls off. The free energy of course, goes larger with temperature negative and large internal energy starts from minus one say in this normalization and it approaches towards a smaller value.

And, the entropy as I said entropy at 0 temperature is of course, 0, but then at finite temperature entropy will just again become S S will become $K \log K B \log 2 J$ plus 1 which is 2 here.

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So, this is what the entropy will approach to. At high temperature, these spins will sample all the possible two states it has. So, total number of states will be 2 to the power N and log of that will be $N \log 2$ and S by N is basically $K \log 2$. So, that is the result that exact solution tells us and it's very very different from the mean field result. The trouble is that in mean field one does not distinguish between any dimensions or anything and it replaces all the fluctuations to 0 it sets all the fluctuations to 0.

And, here in low dimensions is the fluctuation that is very important and as shown by the exact calculation, the fluctuation kills the order and there is no spontaneous order at any finite temperature for Ising model in one dimension. So, that is a result which I want you to remember that low dimensional systems are dangerous because there are there is huge fluctuation and that fluctuation has to be taken into account, if you want to do a theory on to understand those models.