Basic Statistical Mechanics
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Lecture - 46
Ising Model and Other Lattice Models (Part 3)

Welcome back. We shall continue with our study of Ising Model. As I stated several times in the last lecture on Ising Model that this is the perhaps the most important model of statistical mechanics. It serves several purposes. On one side, this is the simplest model of many body interacting system and at the same time, it captures most of the essential features like phase transitions, critical phenomena and many, many other aspects of many body problem.

One thing one should know, remember while doing this that this Ising model is not just a model by itself. It goes on to explain lattice gas models in gas-liquid transition. It goes on to explain many aspects of order-disorder transition in binary alloys. It goes on to be used in polymers. So Ising model has this multivarious things. At the core, however, the Ising model is a very simple thing. It just has nothing but spins.

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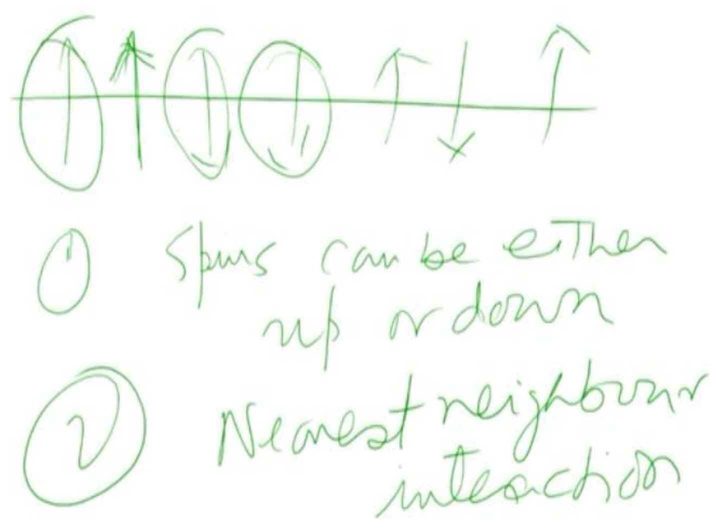

And so I can consider that this is a spin up and down and so the spin is essential element that spins can be either up or down. Second is that this is nearest neighbour interactions. It is very important, that is nearest neighbour interaction. So these 2 are essential parts that mean this guy here can interact only with this one and this one. So this nearest one interaction makes it really simple and one may wonder how such a nearest neighbour can explain so many different things.

The reason is that this is interacting with these, but these are also interacting with this. So the effect of the interaction propagates and the spins can be up and down. They can also flip between the two states. So this is called two-stand Ising model and as I told you before that this is the model, which was introduced by a PhD student Ising in 1925 and he solved it and then, people immediately realized the beauty of this.

However, one-dimensional Ising model does not have a phase transition as we discussed in the last thing. There are two cases that we solved for one-dimensional Ising model and one of them is that in the absence 1D Ising model.

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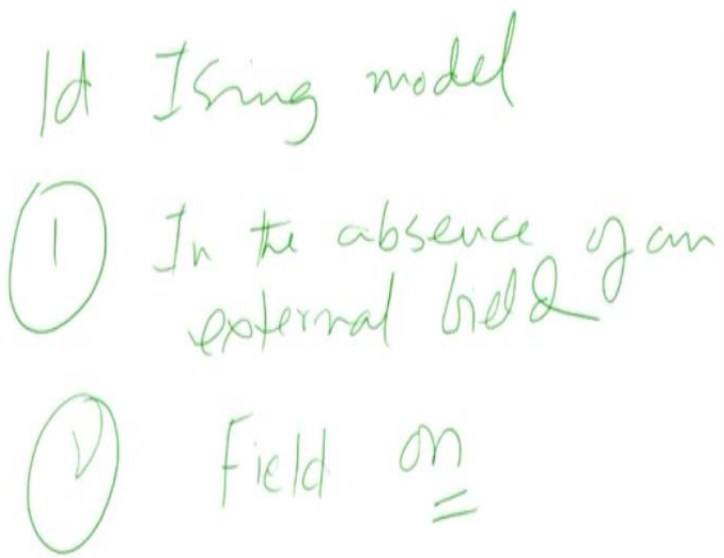

One is in the absence of an external field; the other one we have the field on. Now the solution in the absence of an external field is very simple. We describe it is just

$$Q_N = \left[\cosh\left(2J / k_B T\right)\right]^N$$

That is the simple solution. In the presence of field, the solution is far more difficult, but still analytically doable.

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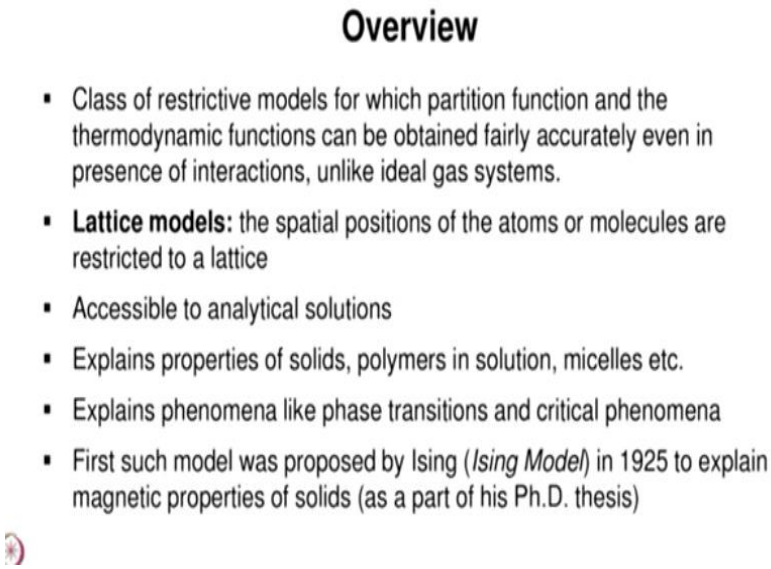

The solution of this one dimensional Ising model.

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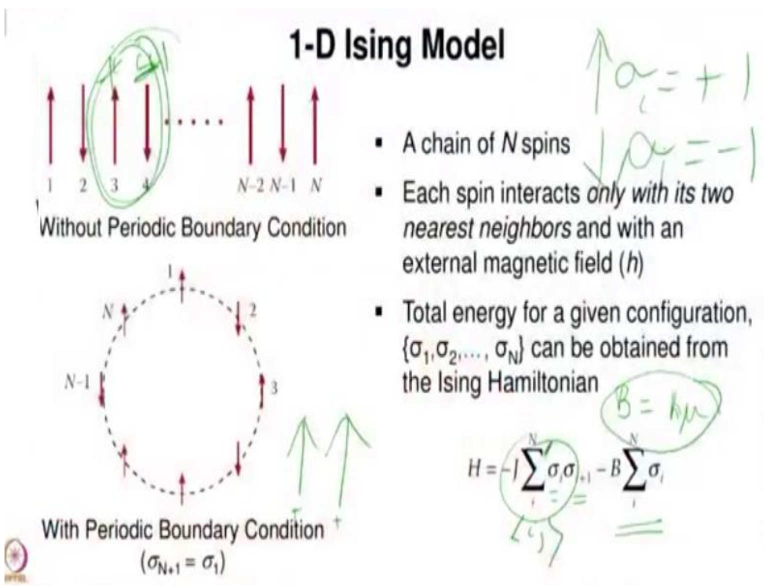

So this is the Hamiltonian of the one dimensional Ising model that this J is the coupling term and so when σ_i can take. The notation we take that when it is up, the spin up, we give σ a value +1. When it is down, we get the value -1 and these are nearest neighbor, so one should really stick to have a thing here that this is saying that these interactions, of course i and i + 1 does that also, the same purpose it does.

Usually one writes something like ij here and then put, because sum is both i and J. That is the other notation that one use, otherwise one can also use this notation. Now if you look at the character of that. So once this i spin and i + 1 spin, this is the i-th spin, this is the i + 1, when both of them rather take, well this is not the best example, but let us see when both are up, then both of them bring +1, +1, then these become –J and when they are down, then again -1, -1, then also you get –J.

However, when one is plus and another is minus like here, then these will be plus and this is minus, this will be plus and this will be minus and this whole thing then contributes, this particular pair continues a minus term and then becomes plus. So when they are parallel, whether they are both up or both down, then they contribute negatively with the total Hamiltonian and that is favorable.

So when two parallel spins are favorable, up and down that is called ferromagnetic interaction. However, when they are opposite spins, so in that ferromagnetic interaction, opposite spins are not favored, because this comes with a plus J. It contributes positively increases the total energy of the system and this is what now is an external field, but B actually has any two terms, one is the external magnetic field *h* and magnetic moment μ.

So B is $h.\mu$ and this is the way the Hamiltonian reduces. This is a very simple Hamitonian. It just takes into account certain favorable interactions and certain unfavorable interactions and then one tends to solve this thing and see what kind of result that comes out. So one dimensional Ising model, as I said repeatedly can be solved exactly and we discuss it next time.

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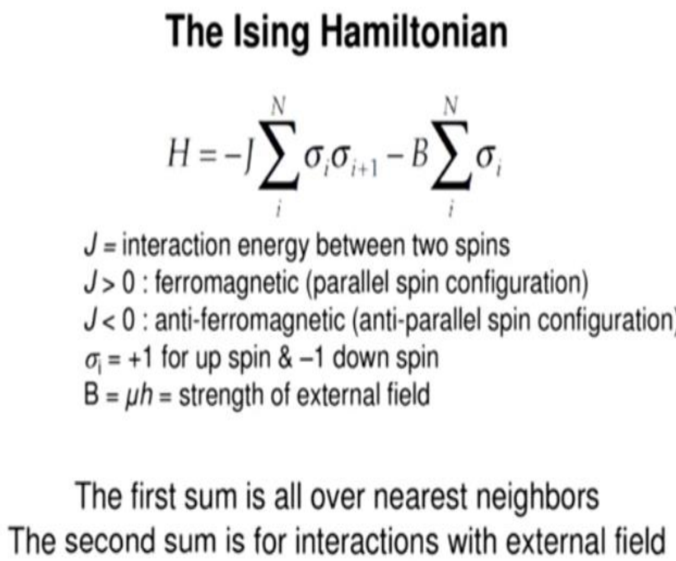

So this is again the Hamiltonian written, all the nearest neighbors and everything.

$$H = -J\sum_{i=1}^{N-1}\sigma_i\sigma_{i+1} - B\sum_{i=1}^{N}\sigma_i$$

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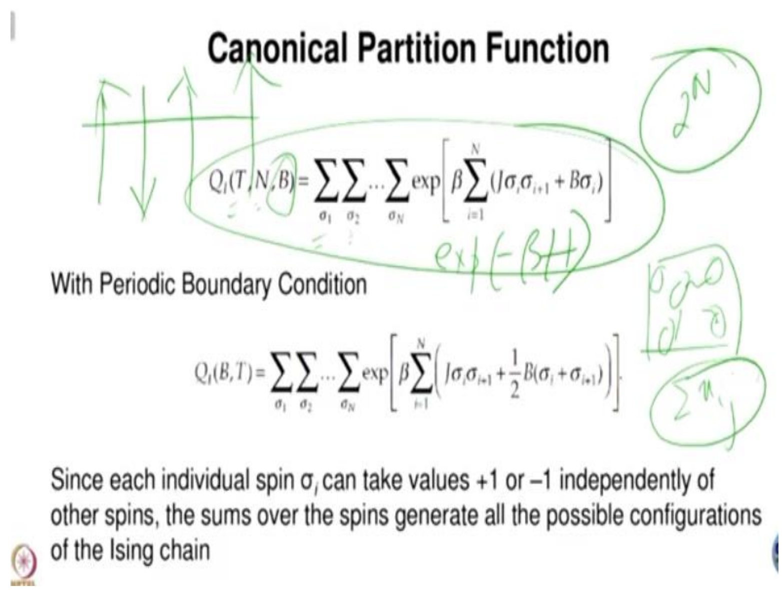

So partition function of these things will be written as the sum over all the configuration.

$$Q_I(T,N,B) = \sum_{\sigma_1}\sum_{\sigma_2}\cdots\sum_{\sigma_N}\exp\left[\beta\sum_{i=1}^{N}\left(J\sigma_i\sigma_{i+1} + B\sigma_i\right)\right]$$

So when you take these sum or all these, so σ1 is plus minus, σ2 is plus minus and σN in plus minus. So you have all in all 2^N configurations. So it is good to do an analogy with gas that we have done. In a gas, if I take one snapshot at a given time, then I have the molecules at different locations.

So the molecules at different locations give a given time at a given configuration of the system. Now, the molecules interact with each other and when the molecules interact with each other, then you get an increased energy and of course, in this case, you have kinetic energy in all case in Ising value, you do not have the kinetic energy, but we have the potential energy and we have discussed at length the potential energy is sum over the pair wise additive term.

Here you have many nearest neighbours in your 3 dimension or 2 dimensional systems and you sum up the potential energy of interactions between them. So a given configuration of a gas or liquid is equivalent to specifying positions of atoms and molecules, at given positions and that in an instant of time, that position is changed and the new configuration is created and your Hamiltonian reflects or captures these change in energy with respect to change in configuration.

So when the system goes to a configuration, which is low energy configuration or favorable, then in the Hamiltonian that is reflected with a low energy or negative energy, which then in the partition function in $e^{-\beta H}$ term, which is here, it will remain as βH term, it has more weight. So all favorable configurations come with a larger way. Let us now analyze how that is affecting Ising model.

In an Ising model with a ferromagnetic interaction, where parallel spins are favored, whenever the spins have a domain when spins are parallel, then that comes with a lower energy. So those configurations, are picked up. So this is the reason why at a low temperature, you get a transition to a ferromagnetic phase. Now one dimension, as I discussed in the last class does not have a phase transition.

It does not have a phase transition, put blankly and very straight forwardly simply because it does not have sufficient number of nearest neighbours. It has just two nearest neighbours in one dimension and that is not enough to give rise to one. There is a beautiful theorem that goes that is, I discussed in my book. I will just refer to it a little bit to Ashcroft-Mermin theorem, which formalizes what I said, that why 1D cannot have a stable ground state or ground energy state, except that temperature T = 0.

At temperature T = 0, β is $1/k_BT$ that diverges, so only this one particular configuration is picked up. So now, the idea is then to calculate in this partition function, but would like to tell you that the purpose of this class is different from the last class. I am just preparing little bit, spending some time to talk about and then go over to what I am going to do in this class. So I write now the canonical partition function, which is the function of the temperature, total number of spins and the magnetic field B.

And that is written instead forwardly from the Hamiltonian, which is given here.

$$H = -J\sum_{i}^{N-1}\sigma_i\sigma_{i+1} - B\sum_{i}^{N}\sigma_i$$

That Hamiltonian is written and gets into this partition function. It is rewritten again essentially for certain periodic boundary condition, which we do not need to discuss now, but it essentially says that you can make it into a ring and that is possible only in 1D, this beautiful ring thing, so that these, these and these spins, it is only one next to that is the same configuration and so make it into a ring that there is an advantage of mathematical representation, which allows us to solve this problem.

$$Q_I\left(h,T\right) = \sum_{\sigma_1}\sum_{\sigma_2}...\sum_{\sigma_N}\exp\left[\beta\sum_{i=1}^{N}\left(J\sigma_i\sigma_{i+1} + \frac{1}{2}B\left(\sigma_i + \sigma_{i+1}\right)\right)\right]$$

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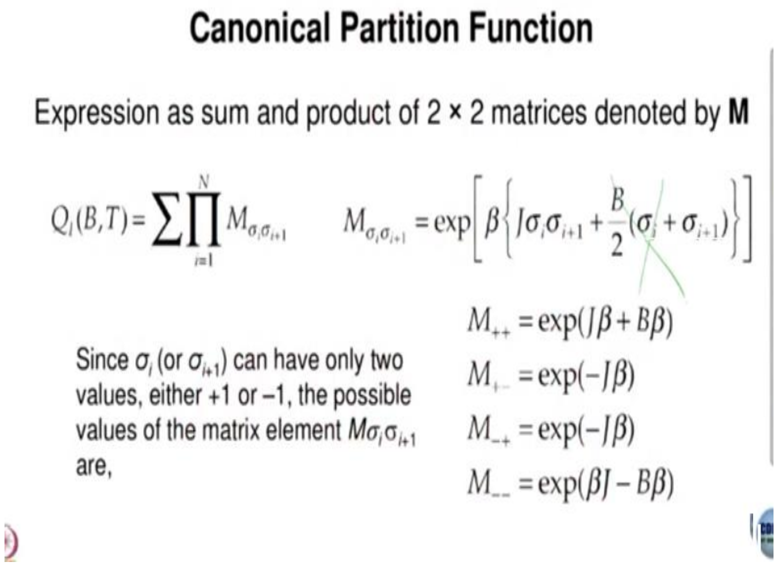

Now, this I discussed little bit that this is solved by making a method called transfer matrices and This is essentially discussed here,

$$M_{\sigma_i\sigma_{i+1}}=\exp\left[\beta\left\{J\sigma_i\sigma_{i+1}+\frac{B}{2}(\sigma_i+\sigma_{i+1})\right\}\right]$$

I do not want to go into that detail, but I solved at length in the last class the case when there is no magnetic field B = 0. When B = 0, then this Hamiltonian, this part is not there. It is very simple. Then, I can show that this will be e to the power –β J and get that goes to be cosh and then you get cosh ($2J/k_BT$) to the power N, that partition function.

And then, one can show that partition function does not have a phase transition, which is similarly, I just tell you with the well know results in this.

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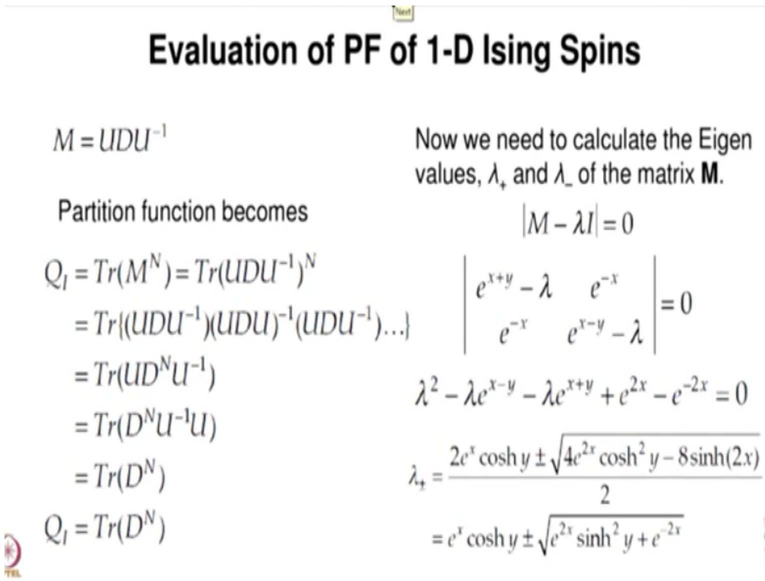

I discussed a little bit in the last class.

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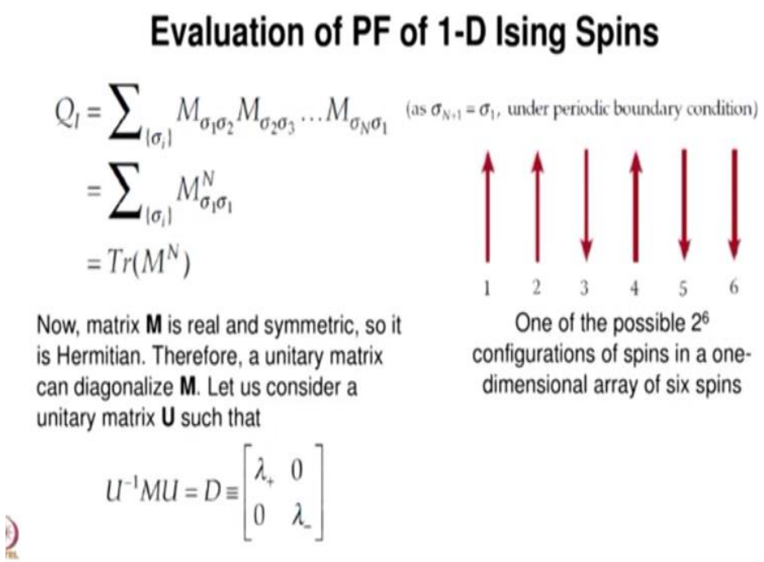

How you go through a transfer matrix, then how you use a unitary, this aims a symmetric matrix, which is nothing but this.

$$Q_I = \sum_{\{\sigma_i\}} M_{\sigma_1\sigma_2} M_{\sigma_2\sigma_3} \cdots\cdots\cdots M_{\sigma_N\sigma_1} \quad \text{(as } \sigma_{N+1} = \sigma_1 \text{, under periodic boundary condition)}$$

$$= \sum_{\{\sigma_i\}} M^N_{\sigma_1\sigma_1}$$

$$= Tr\left(M^N\right)$$

$$U^{-1}MU = D \equiv \begin{bmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{bmatrix}$$

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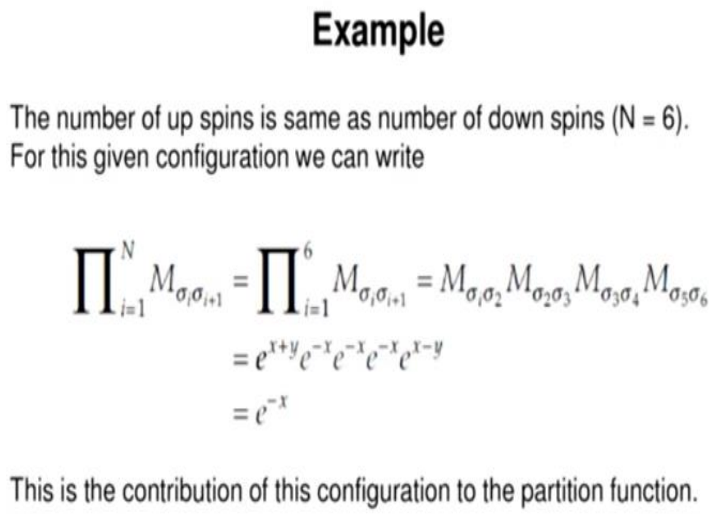

This x and y or β J and β B and the diagonal and diagonal terms, but I do not want to go into too much detail into that today, but I just want to show you the final results of the partition function, which is for the time being for us, this is okay.

$$\prod_{i=1}^{N} M_{\sigma_i\sigma_{i+1}} = \prod_{i=1}^{6} M_{\sigma_i\sigma_{i+1}} = M_{\sigma_1\sigma_2} M_{\sigma_2\sigma_3} M_{\sigma_3\sigma_4} M_{\sigma_4\sigma_5} M_{\sigma_5\sigma_6}$$
$$= e^{x+y} e^{-x} e^{-x} e^{-x} e^{x-y}$$
$$= e^{-x}$$

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Evaluation of PF of 1-D Ising Spins

$$\lambda_+ > \lambda_- \qquad Q_I = (\lambda_+)^N + (\lambda_-)^N$$
$$= (\lambda_+)^N \text{ for large N.}$$

As $N \to \infty$ only larger eigen value λ_+ is relevant, because

$$\frac{1}{N}\ln Q(h,T) = \ln \lambda_+ + \frac{1}{N}\ln\left(1+\left(\frac{\lambda_-}{\lambda_+}\right)^N\right)$$

$$Q_I = \left\{e^x \cosh y + \left(\sqrt{e^{2x}\sinh^2 y + e^{-2x}}\right)\right\}^N$$

$$Q_I = \left\{e^{\beta j} \cosh\ (\beta B) + \left(\sqrt{e^{2\beta j}\sinh^2(\beta B) + \mathrm{e}^{-2\beta j}}\right)\right\}^N$$

$$\left(e^{\beta J} + e^{-\beta J}\right)^N$$

So this is the final expression of the partition function of the N spin in the presence of a magnetic field and if the magnetic field goes to 0, then one can show that this term goes to 0 and you can combine the two things, this goes to 1, and you will get

$$Q_I = \left(e^{\beta J} + e^{-\beta J}\right)^N$$

that is when B = 0, but important thing is that this is already you can see this is considerably difficult and complicated partition function.

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Thermodynamic Functions

Free Energy

$$A_I(B,T) = -k_B T \ln Q_I(B,T)$$

$$A_I(B,T) = -Nk_B T \ln \lambda_+ = -Nk_B T \ln\left[\left\{e^x \cosh y + \left(\sqrt{e^{2x}\sinh^2 y + e^{-2x}}\right)\right\}\right]$$

However, even this complicated partition function, which was derived by Ising many years ago, does not show a phase transition. You can now go and get the standard this ln, you get the free energy from the partition function

$$A_I\left(B,T\right)=-k_BT\ln Q_I(B,T)$$

and that quantity becomes just this quantity. This probably is not needed at this point.

$$A_I(B,T)=-Nk_BT\ln\left[\left\{e^x\cosh y+\left(\sqrt{e^{2x}\sinh^2 y+e^{-2x}}\right)\right\}\right]$$

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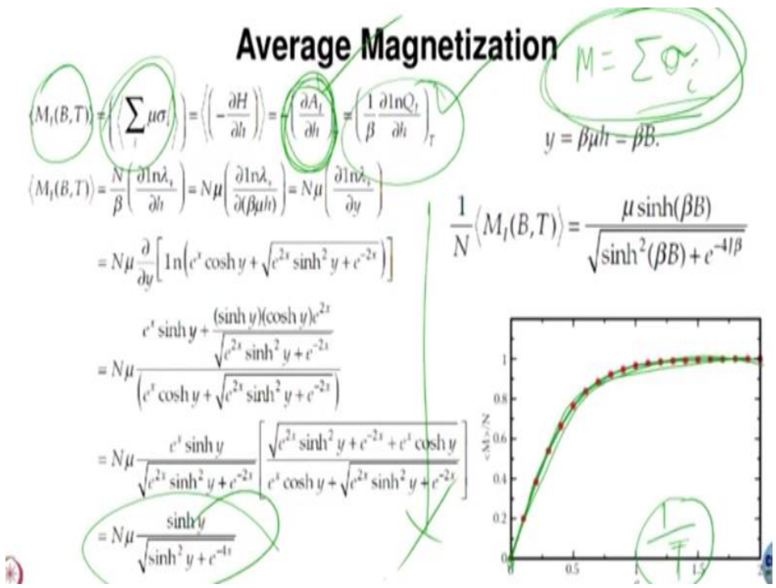

And this term now when you plot and do magnetization,

$$\langle M_I(B,T)\rangle=\left(\left\langle\sum_i \mu\sigma_i\right\rangle\right)=\left\langle\left(-\frac{\partial H}{\partial h}\right)\right\rangle=-\left(\frac{\partial A_I}{\partial h}\right)_T=\left(\frac{1}{\beta}\frac{\partial\ln Q_I}{\partial h}\right)_T$$

$$or,\langle M_I(B,T)\rangle=\frac{N}{\beta}\left(\frac{\partial\ln\lambda_+}{\partial h}\right)=N\mu\left(\frac{\partial\ln\lambda_+}{\partial(\beta\mu h)}\right)=N\mu\left(\frac{\partial\ln\lambda_+}{\partial y}\right)$$

magnetization is nothing but total number of spins, so magnetization is number of spins that are up, so that can be obtained by number of spins up minus number of spins down. So it is just sum over the state of the spins. This gives you the magnetization.

$$< M_I(B,T) >= N\mu \frac{\partial}{\partial y}\left[\ln\left(e^x \cosh y + \sqrt{e^{2x}\sinh^2 y + e^{-2x}}\right)\right]$$

$$= N\mu \frac{e^x \sinh y + \frac{(\sinh y)(\cosh y)e^{2x}}{\sqrt{e^{2x}\sinh^2 y + e^{-2x}}}}{\left(e^x \cosh y + \sqrt{e^{2x}\sinh^2 y + e^{-2x}}\right)}$$

$$= N\mu \frac{e^x \sinh y}{\sqrt{e^{2x}\sinh^2 y + e^{-2x}}}\left[\frac{\sqrt{e^{2x}\sinh^2 y + e^{-2x}} + e^x \cosh y}{e^x \cosh y + \sqrt{e^{2x}\sinh^2 y + e^{-2x}}}\right]$$

$$= N\mu \frac{\sinh y}{\sqrt{\sinh^2 y + e^{-4x}}}$$

When you plot the magnetization against β, β is $1/k_BT$, then you see that when β is 0, at high temperature, up spins and down spins are equally favored.

So you have then up spins and down spins equally favored, this is again equal to 0, which is starting here. Now on the other limit, when T goes to 0, absolute temperature, then β goes to infinity and then as I told, that then the parallel spins are picked up, because they have lower energy, but see the most important thing. The most important thing is that that continuously goes steep.

So this is the very important result that shows that one dimensional Ising model does not have a phase transition. Again the details are done here. As I said that this magnetic field is sum over σ_i, which can be obtained by taking derivative of, and this you all know, the magnetization is derivative of free energy with respect to magnetic field and these are things we have done many, many times and written like that.

Then you can do this little algebra, but even in this case, little algebra is not too little because of this sinh and cosh terms are involved, but this is the final result, that one obtained after doing these calculations here. So this is in the presence of the magnetic field. In the absence of the magnetic field, it is much simpler and you essentially have the same behavior that means you do not have a best condition. This situation is completely different.

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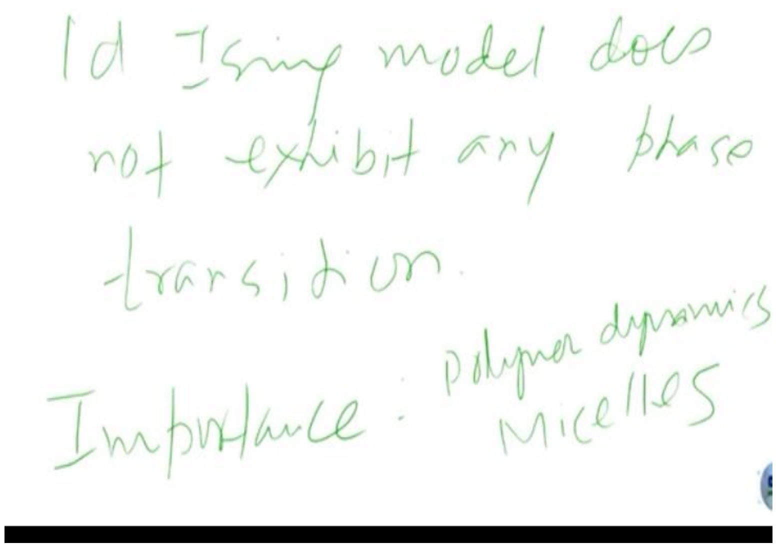

So the 1D Ising model does not have a phase transition. This is a very significant result, does not exhibit any phase transition, but even then the one dimensional Ising model plays an extremely important role. So even then, I will just spend one minute on the importance. This is the model, which is used to do polymer dynamics. It has been described Micelles and reverse Micelles. Many, many models, many, many cases even one dimensional Ising model has been used.

And one of the most successful theory of dynamics interacting system is based on one dimensional Ising model. So now that one dimensional Ising model we read, we know how to solve. I worked out in the last class the zero magnetic field and in the presence of complete magnetic field is fairly demanding calculation, even though it is just one dimension, so I just referred to the book and the transfer matrix method, which you can do.

So now, we have to go to the next case. One dimensional Ising model gave us some understanding of the interacting systems and the temperature dependence, which does not show first phase transition, pretty nice features in many different ways, of course some beautiful solution in terms of cosh and sinh. Now we want to do, okay what happens and that was the question immediately asked after Ising that what is happening in other dimensions.

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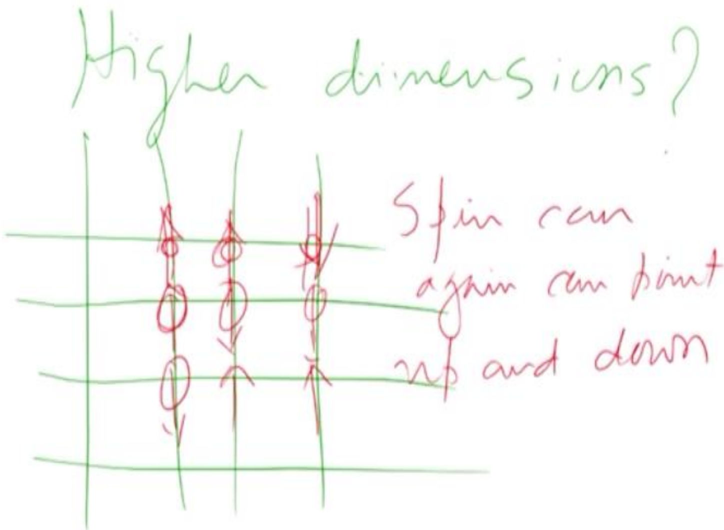

And that turned out to be really, really highly enjoyable, but very difficult journey for physicist and chemists. So the higher dimensions, people, though it was 1925, then it took almost 20 years to get the solution in the 2D. So in the two dimensional Ising model, now we have, say, a square lattice, three dimensional kind of face-centered or body-centered or simple cubic lattice also. Here you have all different varieties. So in this case, what you have?

You have spins in again, up and down, but you have spin at every lattice site. So these arrows are in the lattice side. So you have now a spin on each lattice side and this spin can again do the same thing. Spin can again spin and again point up and down. So that part remains the same. So in the Hamiltonian, we write the Hamiltonian.

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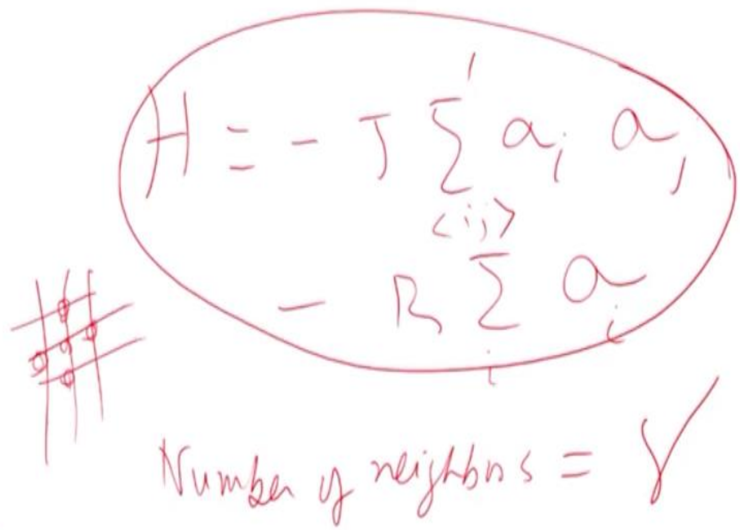

This remains the same.

$$H = -J\sum_{i=1}^{N-1}\sigma_i\sigma_{i+1} - B\sum_{i=1}^{N}\sigma_i$$

So Hamiltonian remains the same, but we are working on two dimension, so i, j and again here is the neighbour. So now in the case of higher dimension, I can say number of neighbours, which is now denoted by γ, in this class. So here then, in my 2D square lattice, I have γ = 4. If I go hexagonal lattice, then I will have a γ = 6. If I have simple cubic three dimensional lattice, then again my γ number may be estimated as 6.

But if I now go to face-centered cubic lattice, I will have number of nearest neighbours 12 and body-centered cubic lattice, I will have 8. So then, in this treatment, in this Hamiltonian, the information about the lattice is coming through the number of nearest neighbours. So not only that we have spins up and down, we will also have the nearest neighbour interaction. So those two basic features of one dimensional Ising models carry on to two dimension and three dimension and it is ready now.

But the two dimensional things are exceedingly difficult and it was solved and it took large number of people tried to solve the two dimensional problem, it was solved by Lars Onsager in 1944 by a solution, which is considered perhaps the most difficult calculation ever done in the history of physics or science, this Lars Onsager solution. But Lars Onsager solved it in the absence of magnetic field.

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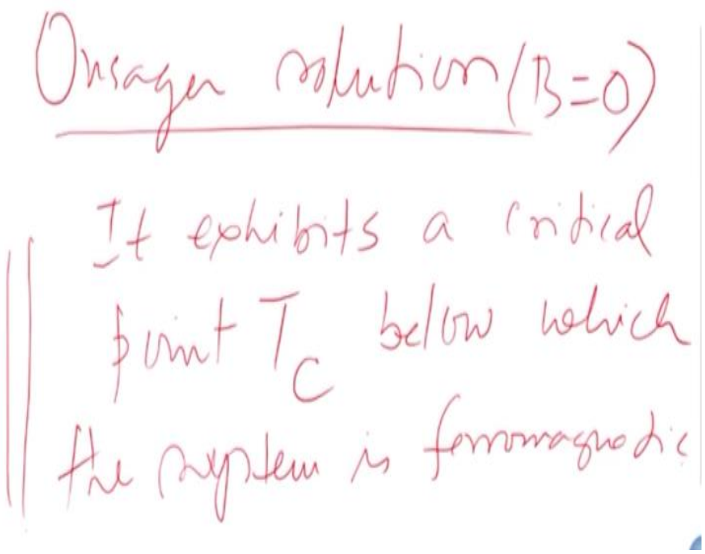

What is the Onsager solution? It is a very difficult solution, but I will say the basic features. It exhibits a phase transition. It exhibits a critical point Tc, below which the system up spins is ferromagnetic and above which it is not. So that is a beautiful result and hugely difficult calculation. The Onsager solution was in the absence of magnetic field (B=0). This was with finite magnetic field was done, another calculation by Yang.

And he found then the other beautiful thing that in the presence of a magnetic field, the phase transition becomes first order and it exhibits hysteresis. So the basic things of magnetic phenomena was captured by the two dimensional Ising model. Three dimensional Ising model nobody has solved three dimensional Ising model. It remains an unsolved problem. People have done huge amount of numerical work.

People verified that much of the features of two dimensional Ising model remain same as the three dimensional Ising model. People have used three dimensional Ising model for experimental systems and it has been found to be remarkably successful in explaining many, many things of people, but the fact remains that three dimensional Ising model, it has not been possible to solve mathematically. Many, many people have tried.

Many, many people, I know, have tried and they could not go anywhere. Two dimensional Ising model itself is very difficult and I can talk you of the solution and I can tell you of the basic features, which is more or less here and there are some many things that really went to critical phenomena that I want to talk a little bit later today that how these things go on. But before we do that, this Onsager solution, I want to go a little different path.

And I want to do something, which captures the physics of the problem that we are trying to deal with, without really doing this amount of work that is required in two dimensional Ising model and this is an approximate method that has been invented over the years and has been successfully employed.

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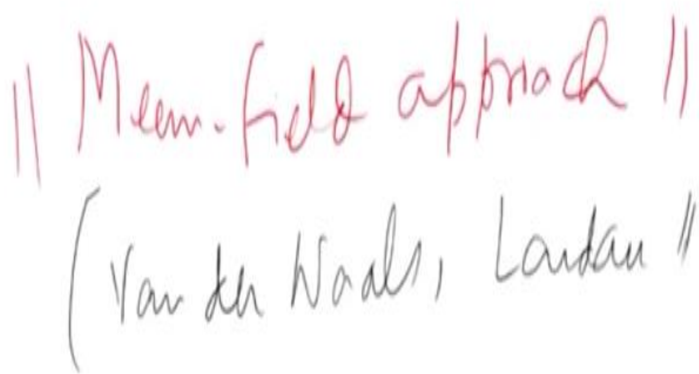

This is called the mean field approach and the mean field approach also goes by many other names. It goes by the name of van der Waals. One can show the van der Waals equation of state that we have studied that van der Waals is essentially mean field, then we have done Landau theory at great detail. Then Landau theory is also this mean field theory. However, what we are going to do today now?

Do the mean field theory in the context of the Ising model and we will get the results of the Ising model. The results are not 100% correct, approximate, but it will capture many of the physics of the two-dimensional, three dimensional system. Mean Field theory is really bad in two dimension. It becomes more and more accurate as we go to higher and higher dimensions and there is always a critical dimensionality, where mean field theory becomes exact.

But in three dimension is bad, but in four dimension it becomes pretty good, so we will now go on develop the mean field approach. The reason we will develop the mean field approach that it has a beautiful insight and very useful insight that it provides in addition to the results, which are highly useful and in more places, routine applications, this mean field theory plays a very, very important role, that is like Landau theory.

And we actually do not go back to a very formidable Ising model kind of compelled interacting system, just like for the Mayer's theory, breaks down to a point, then what we will do? People, of course, try to extend it, like people try to solve three dimensional Ising model exactly and could not do it, but then the alternative approach that appeared is to take on the education for there, but then build a completely different model, like the Landau's theory.

Then Landau's theory wanted to take correlations that how he went on to go over something called Ginzburg-Landau theory. So basically, one takes a step backward and develop an approximate theory, since the really exact path is kind of blocked for you. You can do simulations something, but you are undergoing very analytical one. So in that case, you take a step backward, build an approximate theory like Landau theory. Then go forward to make that theory far more understandable and far more, far more useful. So we will now go to the mean field theory and try to describe what is the mean field theory.