Basic Statistical Mechanics
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Lecture – 45
Ising Model and Other Lattice Models Part 2

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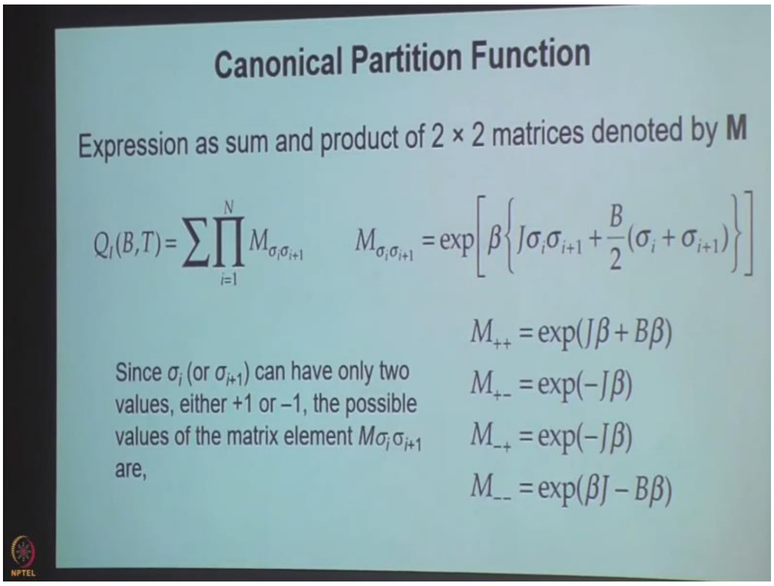

So now the way it is done is to recognize you can go over,

$$M_{++} = \exp(J\beta + B\beta)$$

$$M_{+-} = \exp(-J\beta)$$

$$M_{-+} = \exp(-J\beta)$$

$$M_{--} = \exp(\beta J - B\beta)$$

that you recognize that you can decompose the partition function just like we did. You can decompose the partition function in terms of matrices and these matrices are very simple matrix.

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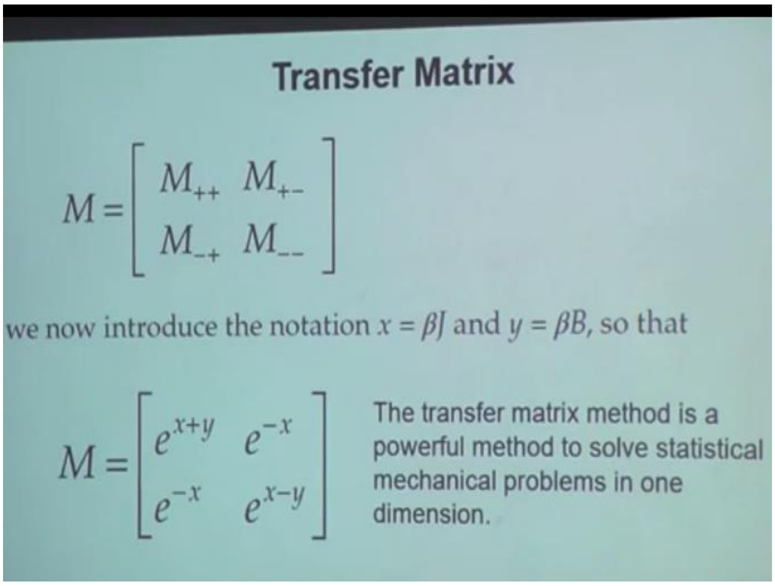

$$M = \begin{bmatrix} M_{++} & M_{+-} \\ M_{-+} & M_{--} \end{bmatrix}$$

$$M = \begin{bmatrix} e^{x+y} & e^{-x} \\ e^{-x} & e^{x-y} \end{bmatrix}$$

These are the matrices that it comes. These are the diagonal terms and you can essentially use these matrix to propagate the nearest neighbour correlations to all order and you do very similar thing that we have done here to the power N, but you cannot decompose completely like that. I have done here because we introduced an asymmetry in the problem. The symmetry that I had in this problem that is broken because of this term.

Because here two down comes with the same term with two up. But here that is reflected here two up and two down are not the same because this B is the magnetic field. So when you are going down, if the spin is up, then both the two spins down will be unfavourable. So that will come as a plus sign. Otherwise both spins up that will come with a negative sign. So these symmetry of this Ising Hamiltonian in the absence of the magnetic field is broken as it should in the presence of the magnetic field by this term.

One can solve this, let me tell you that by transfer matrix method, we did diagnosation. The reason of my not doing it, it uses some theories of Eigen value analysis, which will take a long time to do that I am not going to do.

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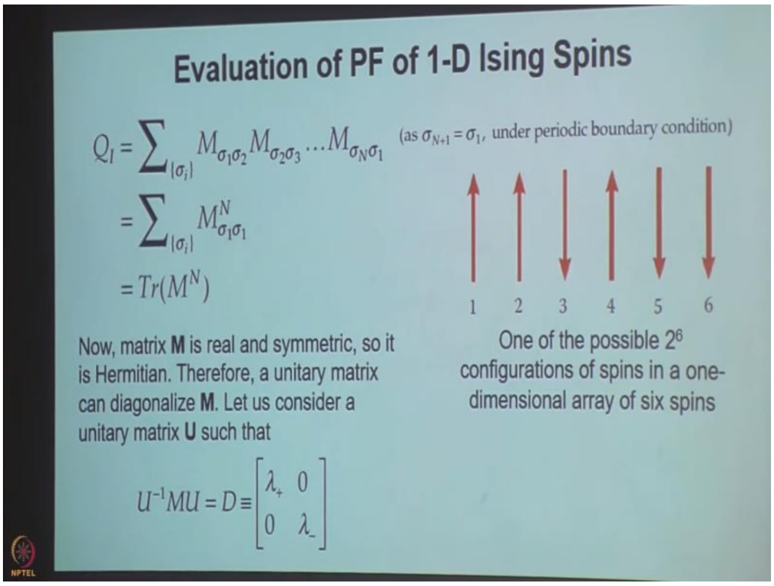

But I will tell you and there is some examples done.

$$Q_I = \sum_{\{\sigma_i\}} M_{\sigma_1\sigma_2} M_{\sigma_2\sigma_3} \cdots\cdots\cdots M_{\sigma_N\sigma_1}$$

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

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

If you will see that particularly what happened when you have these kind of spins which are kind of things that I have a little better than how configurations gets energy and how you can calculate the Eigen values of such things,

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

but let me tell you the result.

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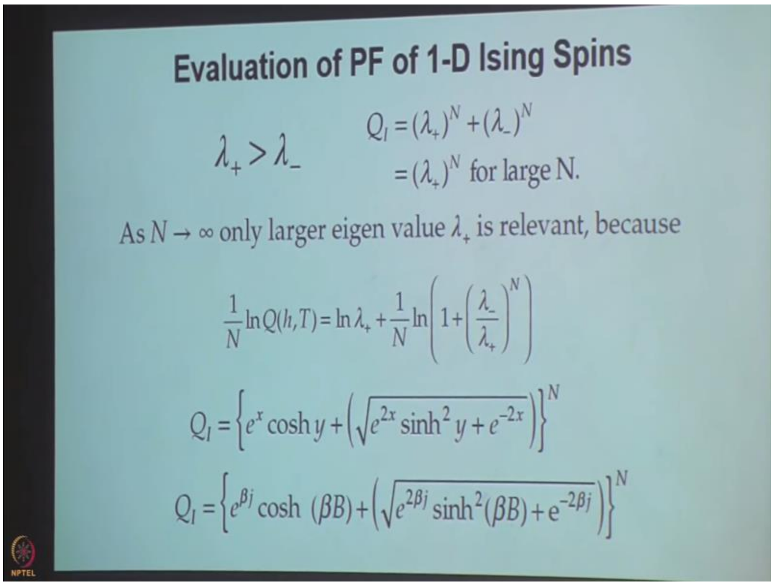

This is interesting but not almost the same kind of thing that we have.

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

So this is the partition function now. That is what I was saying. It included the calculation of the Eigen values which you will find most of the books and I assume the Eigen values of this matrix. This matrix, you have to find the Eigen values of that matrix and then you notice that one Eigen value is larger than the other Eigen value.

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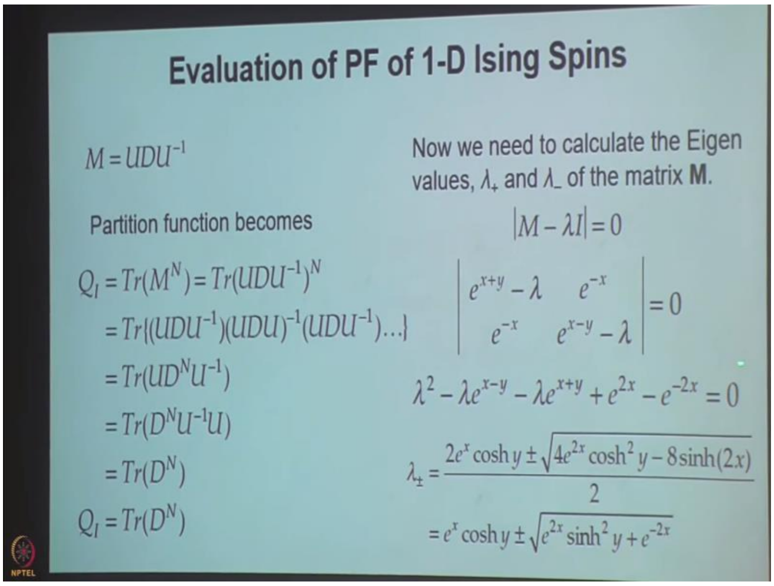

Then, like here these two Eigen values analysis done here and one is larger than the other one. So in the end going to infinity, one of them remains but let me tell you the basic result. The final result is, this is the partition function Q_I for Ising in the presence of the magnetic field is a considerably more complicated but still analytical equable. You can go through this. This have to be done analysis then you have to do certain, it is not too difficult.

$$Q_I = Tr\left(M^N\right) = Tr\left(UDU^{-1}\right)^N$$

$$= Tr\left\{\left(UDU^{-1}\right)\left(UDU^{-1}\right)\left(UDU^{-1}\right)\cdots\cdots\cdots\right\}$$

$$= Tr\left(UD^N U^{-1}\right)$$

$$= Tr\left(D^N U^{-1} U\right)$$

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

$$Q_I = Tr\left(D^N\right)$$

Very similar thing that we did in the absence of the magnetic field, same factorization and then we sum over all these things. This is the theorem I was saying. I am not comfortable whether that quantity is the trace of M to the power N and then of course you have to have certain kind of imitation in the symmetric matrix. The unitary transformation of the symmetric matrix and the partition function come as this diagonal matrix, diagonal to the power N.

And then that is this to the power N. This is the diagonal matrix 2 to the power N, which is exactly equal to that. So I do not want to go through all these. These are mathematics thing you can do and they are not difficult mathematics, but you have to do that. It is all given there. So the partition function then becomes this thing.

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

Look at that how much more complication, we have when the electric field and magnetic field is there. Then you go to if i would be equal to 0, then it will go over to the old form.

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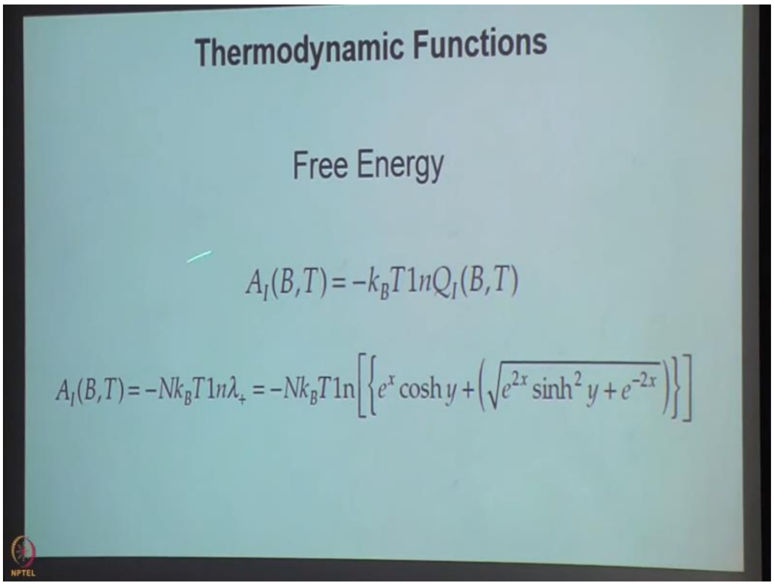

Then we can calculate the free energy,

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

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

using that Ising and then you can get, as they said one of the Eigen values survived because other ones is small. So N going to the infinity limit this is very easy with respect to that one. These are the asymptotic analysis and then you get this free energy. This is very interesting. Once we have free energy, then we can do some work with that.

We could not do something over there in the earlier one that I have worked over here because we did not a magnetic field. I l could have that to entropy and I could have done specific heat, but I could not do the most important thing that people want, which is the magnetization. But if I have the free energy, I can do the magnetization. Now can you tell me how to get the magnetization from this free energy?

I know I have dumped in some equations on you, but they are not really very difficult, beyond what I have done here was the tricky little thing. After that it is same, though you have to do the unitary matrix transformation, your Eigen value analysis all these things more than what I used to do. When I have to free energy, how do I get the magnetization? Yeah, so all I have to do dA_I/dB and I get the magnetization. That is done here.

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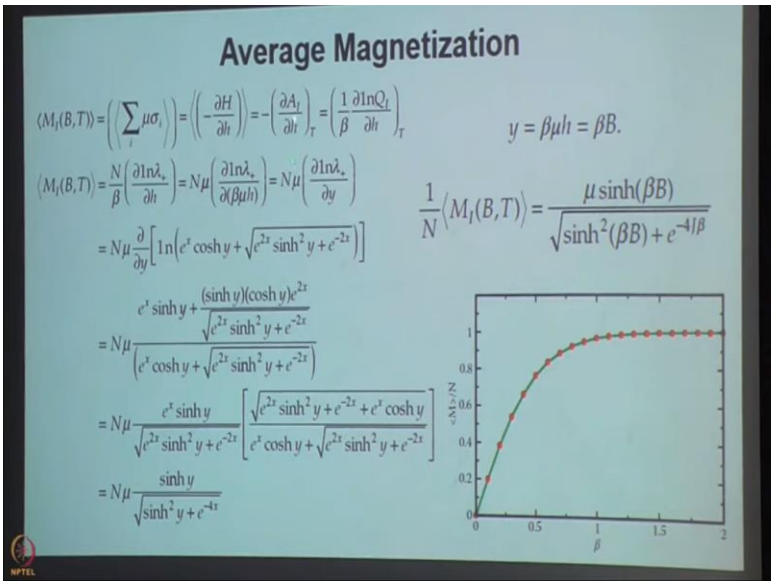

$$\langle M_I(B,T)\rangle = \left(\left\langle \sum_i \mu\sigma_i \right\rangle\right) = \left\langle\left(-\frac{\partial H}{\partial h}\right)\right\rangle = -\left(\frac{\partial A_I}{\partial h}\right)_T = \left(\frac{1}{\beta}\frac{\partial \ln Q_I}{\partial h}\right)_T$$

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

Then magnetization is this magnetic field and H is same as B, magnetic moment taken out. So this is then this quantity. Then one can calculate going back to same as if this lambda plus and all these things and then you get all that, or combine this as y and then we have taken with it through magnetic field and that is why you have to take care of the magnetic moment. We come here and there, change the variable.

I have to absorb it here because this is the quantity that I need as magnetization. I want to go back the variable I have in my work, which is this y and y is this quantity beta B and then I can take the derivative. These are the ugly things that one does not want to do in the class. What you can do? Virtually, it is done there. So I can do the derivative of this Ln. So this comes in the denominator and you take the derivative and will get the terms.

Taking derivative of cosh and all these things is certainly not the most pleasant thing in the world. So because these are two terms there, when you get to it but essentially I think everything is clear here. Nothing should be complicated. Doing in the board is complicated, especially sign. I am mortally afraid of signs. Now we get this beautiful expression. However, at the end of the day you can simplify that.

That remains, these remains and this gets simplified and I think we have to define variables as x, not x, p and q and again do that and this should become the same as this. I think we have to think of. I have to go back e to the power x and e to the power-x, e to the power y and e to the power -y and square all this thing, then we have to combine term. I think here also you have to combine terms. These and this is the same and that is different from this one.

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

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

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

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

But whatever these and this is the same. So I think there is certain manipulation one needs to do that I am not down there for a very long time, but you can do that. But at the end of the day you get the magnetic moment, which is experimentally observable quite easily in these magnetic systems, you get a completely analytical form, that is the main thing. That is a sinh and sinh is as analytic as cosh, hyperbolic cosh.

Now I plot that against one more temperature. Now if there are phase transition what would I expect. I am plotting is 1 over temperature. So this is the high temperature limit and this is low temperature limit. If there is a ferro-magnetic transition, then what will happen? Now tell me what is the ferromagnetic state? Tell me what is ferromagnetic state? See one of the reasons that physics course they learn it very quickly, very rigorously your first year.

You learned it but not in terms of spins in your schools. They should have taught you in terms of things. They need not solve the Ising model but they should have told you about the Ising model. But that is not done, not in Indian context. But Ising is a very beautiful thing and this little thing, I did here I could have been done in high school also. But it does not matter or this solution. Forget about that what has not been done not done.

Now tell me what the ferromagnetic state is. See we are doing phase transition and now the most important phase transition is the magnetic transition, then metal-insulator transition, which is huge amount of industrial arms from that, then semiconductor, superconductivity. Did anybody teach you magnetism? Magnetism has not been taught at all, but in the Integrated PhD it has not been taught yet. They should have taught one magnetism course.

It is of course electrostatics magnetism, because we had that a little bit in our honours course. We had it one small, a half of a course in Calicut university magnetism and then I took lot of courses there for physics department, but I tell you that it is really rewarding. Those of you going to material science and physical chemistry, I hope some of you are going there, because it one of the most fascinating area now and let me tell you organic chemistry is not that fascinating area.

What is going on and on and on the same kind of synthesis. You can get some job but that is very boring. Now so most exciting things are happening at the world of material science and world of biology. Material is particularly exciting. Now as you can see, your TV getting changed, your mobile getting changed. Every technology is getting change in every 2, 3 years. Huge amount of work going on. You know the company IBM, Samsung, you should read more about this. Now the artificial intelligence is getting integrated.

Ferromagnetic is that when all this spins are parallel to each other. That is the ferromagnetic state and paramagnetic state is that when the spins are random. So ferromagnetic state is the state we call ordered state and paramagnetic is the disordered state. So what we are talking of an order disorder transition. It is a very important thing. Please write it down. Order disorder transition is an example of order disorder transition, which is same a melting.

Which is same when you have a beta brass, which I believe is zinc and copper and that undergoes a fabulous transition with a huge change of material properties and we use that material properties many times. You see when you use the safety valves, that we put an alloy and a little change of temperature changes the properties of the alloy. That is the basic of this, when you default in this complex systems.

So these are important thing to know, because chemists make these things and then we just give it to for theoritists to do everything, that if you understand we could have make much better material probably. So apparently the order disorder transition then what would happen in a real system. You would see that there would be a hysteresis. There would be sudden jump of magnetization, this is 1 over temperature. So it will be other way around.

If I put temperature, it would be like that. Otherwise it will be like that, go along like that, so in these systems so the hysteresis and another I told you for system that shows hysteresis is the first order phase transitions. However, the beauty you see in a two dimensional system that even in the absence of the magnetic field, there is order-disorder transition where the specific heat compresses the magnetic susceptibility, so that diverges.

That is the characteristics of order-disorder or a critical phenomena. So the one of the thing that Ising model can use us and that I am going to use to take you to a critical phenomena. So before we go, so this is, as for one dimensional Ising model goes. I have derived a part of it, the basic thing and I have, it is given here. We put it in A. If you want to make it little changes, I would probably make little changes on this chapter and send it to you.

But you can see there is a unitary transformation going over to diagonal and 2^N is λ_1 , λ_N and here you have to work it out. Find out the Eigen values and here the same thing I have done, exactly same thing does here that you go to a factorization. The same factorization comes here that allows me to write it in tutorium. Same thing tutorium, I wrote here. But then you have to go back in analysis. I could sum it up here because I did have this symmetry which is not here.

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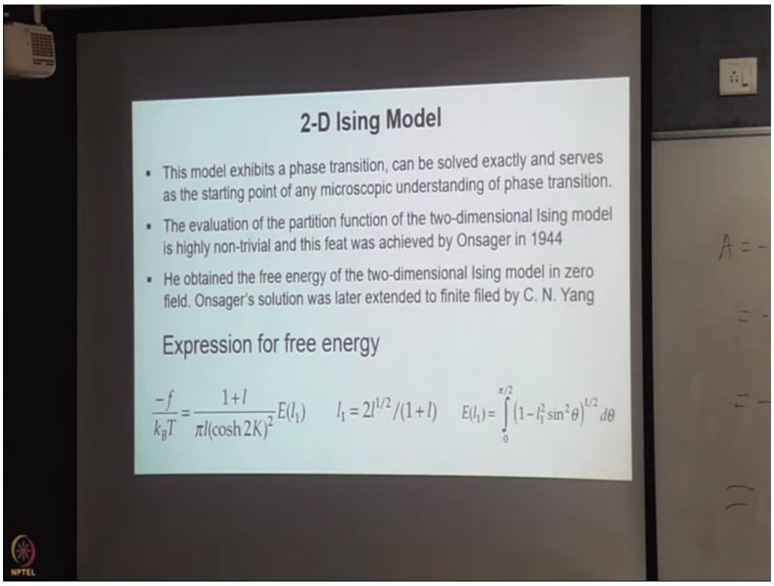

Now these are a hugely important thing an extremely difficult thing at the same time the two dimensional Ising model. I will just tell you the result now and I will do something else which I want to teach you something else, which is the other part of Ising model. Many other techniques which are very useful. So but let me continue a little bit is two dimensional model. I will come back to the two dimensional model.

In a normal course of event I would not have two dimensional model at this stage. I will have a little later and that is what the way I did. So two dimensional Ising model when I have a square lattice and I put the spins. The beauty of this is that this model exhibits phase transition and this played a very important role. As I told you, almost whole history of science that can be solved exactly and it was done by the evolution.

The partition function is extremely highly nontrivial.

$$Q_N = \sum_{\phi_1}\sum_{\phi_2}\cdots\sum_{\phi_m} V_{\phi_1,\phi_2} W_{\phi_2,\phi_3} V_{\phi_3,\phi_4} W_{\phi_4,\phi_5} \ldots W_{\phi_m,\phi_1}$$

It was achieved by Onsager, it is still considered the most brutal and difficult calculation done in the entire physics and that has a very complicated thing in the functional which we are not going to do, but the most important thing that as this magnetization.

$$M = (1-l^2)^{1/8}$$

This is the model shows and this is what you see in experiment.

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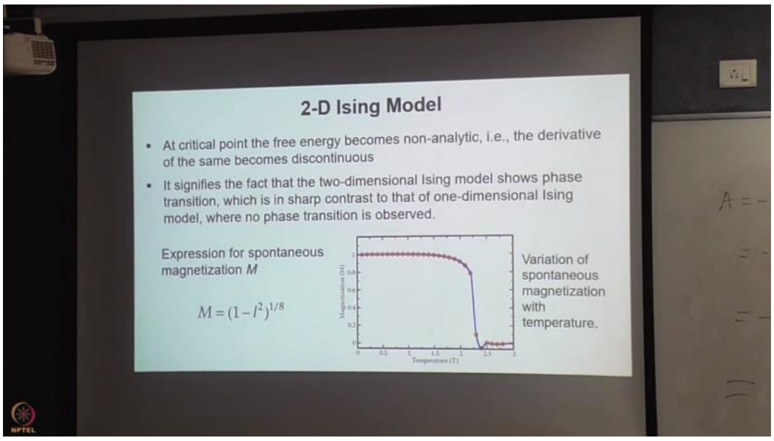

And this fall has certain exponents which is called critical exponents and that is the critical phenomena that we do a little later.

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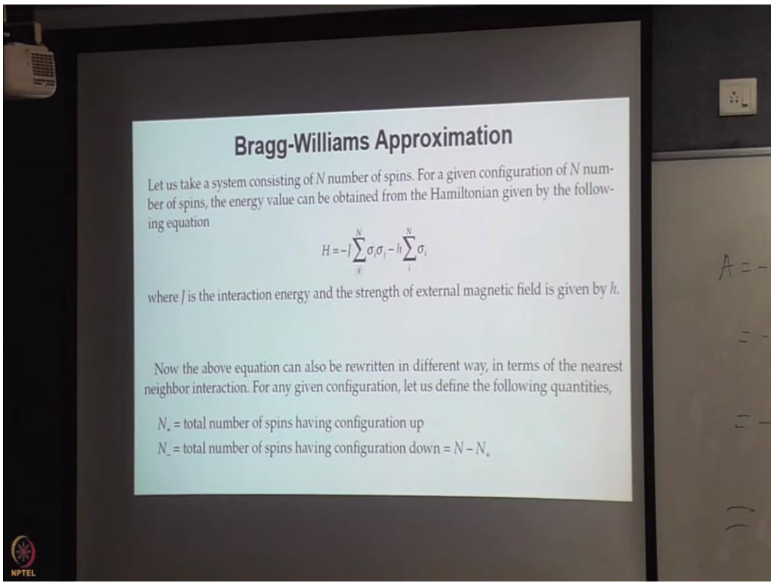

Now, I want to do not the solution, it is a highly nontrivial solution, but I want do now and this is what I want do now and I want to start this. There are certain ways. There is a very important thing in magnetization which is the Curie point. Now can you tell me what is the Curie point? I really strongly recommend that you guys. I will send you some material but you read up in magnetism. It is really not fair not to know about magnetism.

That is not fair. Even if you were doing and this integrated phd students are after all doing PhD, right and you would need. When you are doing organic chemistry, magnetic properties you have to study and many of the things, my magnetic board is organic materials or thing that do you know why magnetic is so important, magnetic properties are studied. The reason is that sometimes you have you do not pair or some characterization you need.

So you need to know the basics of magnetics. So we will make a beginning. This is what the way I will go now. Let me write down and I will come back and forth few things. You should certainly do both of the derivation this will take time about an hour.

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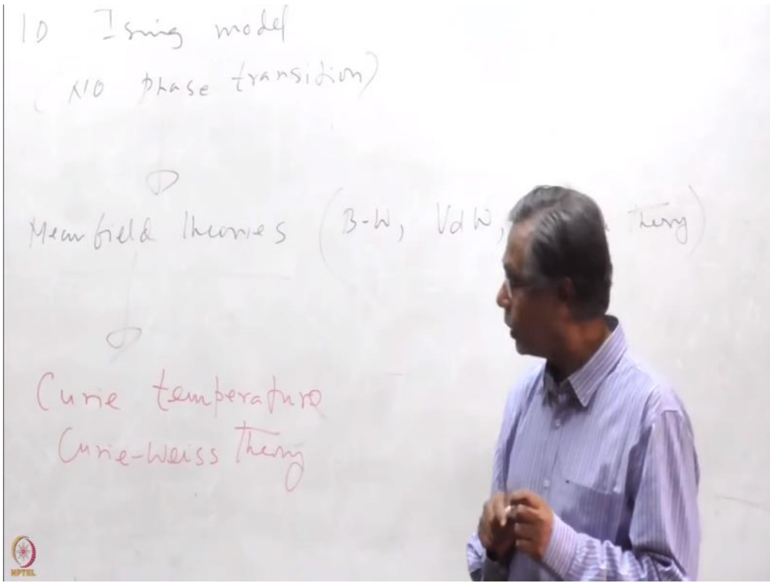

So the flow that I am going to do is we have done one dimensional Ising model. We will not do and we have done the magnetisation and everything and show there is no phase transition. There was a little bit hint of that. Why it is the phase transition that we will come back later, essentially because the new phase cannot be stabilized with only two nearest neighbour and next what we will do is called mean field theories and huge list here in this context of lattices Bragg Williams.

Then this is same as van der Waals, much simpler and more elegant way is Landau theory. Landau theory, we did not do Landau theory here. So we will do the Landau theory after we finish these things. So in the mean field theories, is you have done one example of mean field theory, that is what I was asking, Curie temperature of the molecular field. What is the Curie temperature and also called Qic in equation, what is that?

$$M \sim \left(1 - \frac{T}{T_C}\right)$$

Remember that the magnetisation goes to 0. For magnetisation goes to 0 with exponent 1. If I go $T=T_C$, then T - T - 1 and that is not correct. People found that we saw that 2D Ising is a very different experiment. So the Curie theory, why it was developed we will see that was a mean field theory. Mean field theory is the following concept that it is a very important concept.

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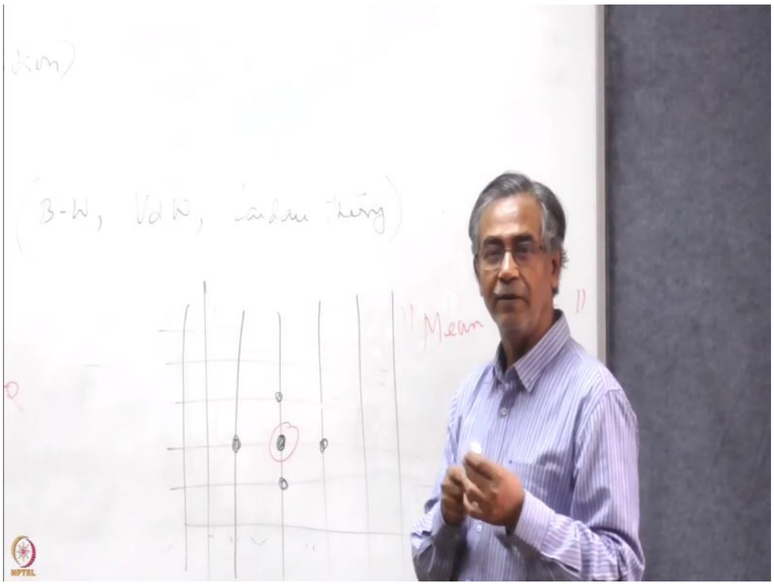

But fortunately they are understandable in a very simple physical way and that is what we do and you will like the Bragg Williams. I am not bragging but I once had the good fortune to teach at Harvard, a really formal course, a course like that stat mech and there is great hall called Pfizer hall where many great people were present with the result I did. There was Bob Woodward's laboratory.

When all the legends are there, but when you teach at that hall the beauty of that is that. When I go to teach, I used to teach from 11 to 12 three times a week. Everything is pakka. There is 9 screens, one screen can be taken out and 9 boards, 9 boards in the following sense in three rows, three column and you start from one side to this to that and three goes on. We press and then one, but more important that is not.

But what I am saying when you enter the second day I told the secretaries in the morning, I want my coffee for me and my students. When I reached, so there was coffee there and everything was clean. All the chalks were ready you know that is what the secretaries are supposed to do. Here god knows what the secretaries do. Most of the time, they do not do anything and we have not assigned job to them.

So coming back, now I have got something nice. I complained a lot but things improve by complaining only. So mean field, let us take nearest neighbour. I have spins here, spins here, spins here, spins here and these are first nearest neighbour and second nearest neighbour are these 4. Now everywhere there is spin and spins. So what is the main effect of the other spins on my central spin think a little bit. This will be continuing with the class.

So let us consider a very high dimensional solid higher than three dimension, then but you know in your mind you can consider. Then number of nearest neighbour increasing. Here I have four, 3D simple cubic it will be 6 like that, now the mean field. I can have a magnetic field or not have a magnetic field. These spins are what are they doing on this. They are interacting. How they are interacting? They are interacting third moments.

Now for a moment if I say I freeze this one, then I will add the effects of all these things. What my spin will see then. My spin will see an average effect. So that is average and mean is the same right. So then I will have my spin here is seeing a mean field. So if all of them are R, then my spin here will also want to be half. So now can I take a description little bit coarse grains opaque description, little bit, not completely microscopic, little bit less like we call it coarse graining.

Where I would be able to talk of the, I write Hamiltonian now in terms of the mean field. Now what I do? These guys also acting on that time. I can construct another way and I can be make them self consistent that is one probably layer up a theory. So this is the way one can get beautiful solutions. So for the phase transitions, we do not have to do as much work and I told me three dimensional Ising model we cannot solve anything.

What do you do what has been able to solve, but you will see this is just like Van Der Waals equation. So we will do these beautiful mean field theories. They are the very favourite of people because this is much easier to do the calculations and much easy to apply. Otherwise, you have to do this in three dimension and this mean field theory is, as I said very favourite us and we continue with that in the next class.