Basic Statistical Mechanics
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Lecture – 44
Ising Model and Other Lattice Models (Part 1)

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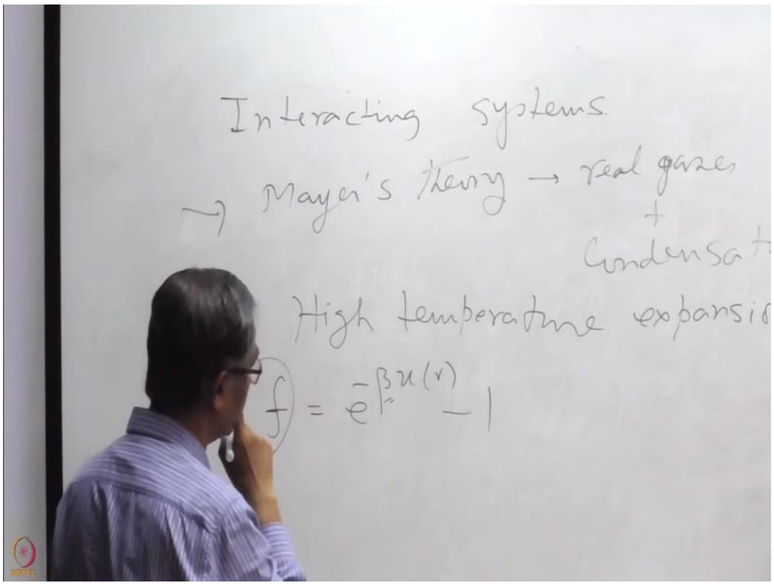

We are trying to do interacting systems where molecules interact with each other and we have done Mayer's theory, which give rise to many other theories but that is essentially theory of real gases and condensation. But that something I forgot to tell is that this is we did it. The reason of that, that it breaks down at high density. But it is more famous in physics. This subject is approached by chemists and physicists in a very different way.

This is called high temperature expansion. The reason is high temperature expansion if you look at it that Mayer function

$$f = e^{-\beta u(r)} - 1$$

So when more temperature becomes large, beta becomes small. So f becomes small.

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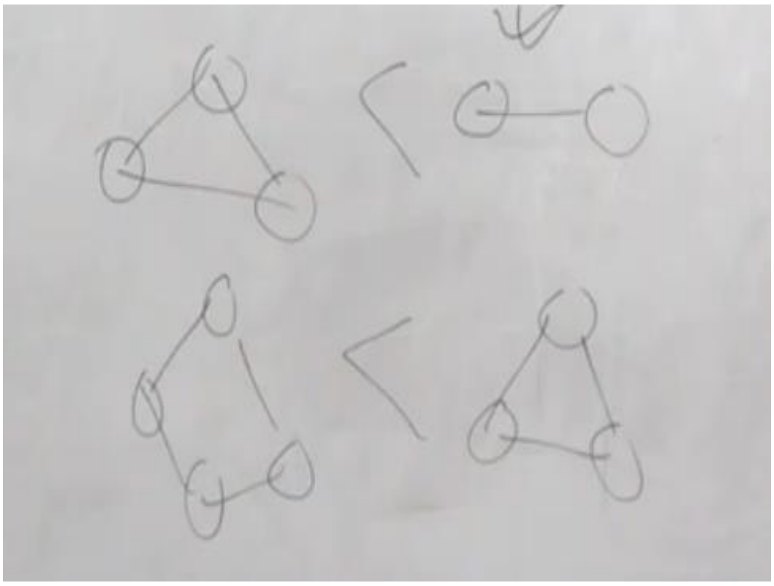

So these kind of graphs that becomes less important than these and then these become less important than these. So at low density of gases anyway, this will be favoured over these, because there are not many molecules per unit volume and these will be more favoured than that. Though it will be larger which will be picked up through, when you calculate the partition function, the cluster integrals and irreducible cluster integrals.

But equally rigorous way of saying that the Mayer's theory essentially and high temperature expansion and viral series is a series in density, but it can also be considered as high temperature, because the higher viral coefficients rapidly decrease with temperature. So that is a different view which comes from $\exp[-\beta u]$ and this high temperature expansion for which all through statistical mechanics simply because of the Boltzmann factor.

So the difficulty comes in statistical mechanics because of the interaction between particles and we cannot evaluate the partition function. We cannot evaluate the total number of microscopic states. And that is why these few cases we can do, rigorously plays a very important role, because they guide us and they provide us insight. Just like Mayer’s theory went on to tell us what is the virial series and went on to develop many other things.

Like I told you sol-gel transition, percolation, the clustering phenomena, the cooperativity just I explained. This is a beautiful phenomenon that you can have. There is an intermediate sized clusters say you can have particle hundred. You can have 50 monomers and dimmers, but other 50 particles can be distributed among the clusters which is 5 of say 10 particles.

Now when you increase the one or two more particles, these large particles can get connected because another particle can come in between.

You can imagine it easily in a lattice in your cell that there are these clusters which are connected. Lattice size another big lattice size and then there is an empty between them. But as you increase the probability of the density, probability of finding a particle, which is mass density then that can get connected. So what happened, in a very infinitesimal change this 5, 10 mers can become 150 mers and suddenly this intermediate size clusters disappear from the system.

And that is what happens when the rains. Say after rains the clouds all the things comes out and sky become clear and you do not see any humidity beyond the point goes down and everything at least upper atmosphere. So this is the same thing the cooperation. So in that sense Mayer's theory is a great theory and give a lot of things but it also has its limitations. As I said that it cannot be pushed beyond the point where everything diverges and extreme low temperature and high density.

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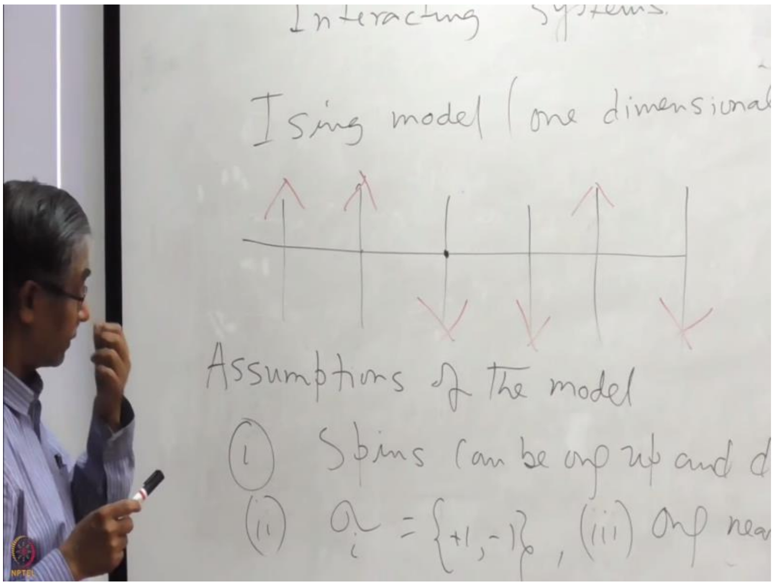

With that cavity, we will go ahead and do the next thing. So second interacting system which of great use in statistical mechanics and find great use in phase transition and because it is solvable in certain exact in certain limits it can be solved exactly it plays perhaps the most important system in the entire physics and chemistry of interacting systems and this is the Ising model. Ising model is a simple one dimensional.

Ising model is also same thing is there for two dimension or three dimensional but they are called two dimensional, 2D Ising 3D Ising. But the original Ising is 1D and then this is essentially you have a one-dimensional chain or odd and you have the spins. Each are spins, so you can take them dipoles whatever and they are interacting with each other. So they can be parallel, anti parallel.

So definition of Ising model is that it consists of spins. Spins can take only two directions. So let me write down the assumptions of the model. One, spins can be only up and down and they are denoted by +1 and -1, as if +1 and -1 comes to a great extent from the logic that you have an external electric magnetic field, so these are in the ferro-magnetic systems. You have an external, so it goes over electrical systems. We use that in real dipoles.

So now these spins can be up and down and they are denoted by plus and one and the variable that comes is σ i and σ i can be +1 and -1. If it is +1, it is up, if -1 is down. And what I stopped telling in a minute ago that why this is chosen, essentially because you have a field in mind and cos θ and so up is this field is aligned on the top. That is just a nomenclature. You can do it any division you want.

But up and down can get in Ising model. So it is cos θ and cos π, so +1 and -1. That is the logic of these two things. Then number three, a very, very important thing that I have only nearest neighbour interaction. That means this spin here can interact only this one and that one. So in a finite spin, when we want to finite change, we know what to do. So in order to reduce the effect of the boundary, we impose what is called periodic boundary condition.

That means we form a ring so after that it becomes this one. This beauty boundary condition which is used in many, many areas in chemistry computer simulations. That is not the part of the assumption. The part of the assumption are these three. The swings can be only up and down. So you do by plus and minus one and the only nearest neighbour interaction is taken into account. So given that you would imagine that is a trivial thing to solve, but it turned out no. It is highly nontrivial.

Nobody has been able to solve three-dimensional Ising model. They are at one time there are sporadic claims. So three-dimensional Ising model but has not been able to do. People have tried, nobody has been able to do and the 2D Ising is very exceedingly difficult and still called the most difficult calculation in the history of physics and that was done by Lars Onsager, physical chemistry, very interesting. So we go now write down Hamiltonian, what is called Ising Hamiltonian.

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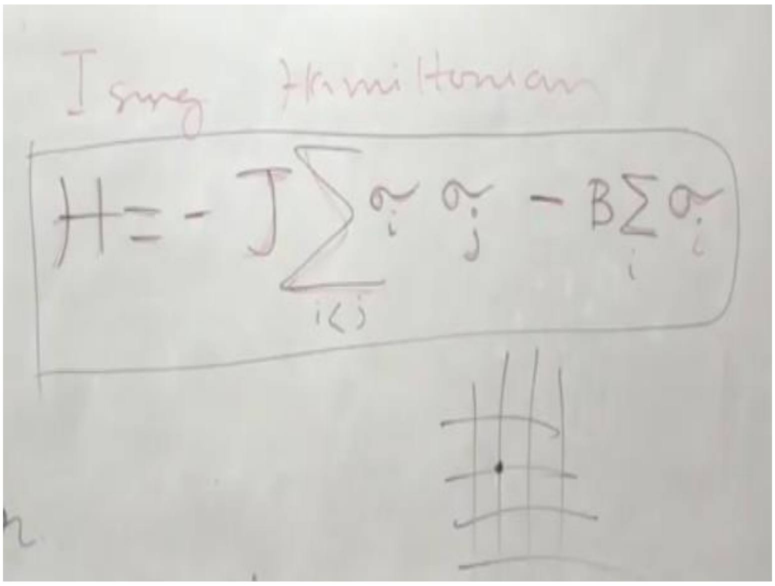

That we wrote down the other day H equal to, let me write down the a one then the general one.

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

So I now spend some time on this. So this is a generalized version of Ising model where the interaction depends on the location that means this interaction can be different from this interaction. So if I call that 1, 2, 3, 4, 5, 6, then 1,2 can be different from 2, 3 and this plays a very important role later, but not we do not need it.

So we consider them to be constant and take it out, so j. So this is done such that when these are both up or both down then I get plus for both of them and then it becomes minus and that is favoured and that is called ferro-magnetic interaction. When parallel spins are favoured. Similarly, negative one, but however is the plus and minus like in this case or in this case you have one plus, one minus and so that becomes -1 and this becomes plus, so that is known term.

And now this is the magnetic field. So magnetic field now, if again in a matter of convention. These are all matter of convention, but they are perfectly general. You can change convention. If you do not like this convention, the result will not change. So this is a magnetic field that is acting on it which absorbs in it to combine the dipole moment or magnetic moment of the spin and the external electric field.

That means a magnetic field is h and in magnetic moment is μ then
B=μh.
So that is combined in that. The effect of the external field is important. Of course, you can have statistical mechanics in the absence of the external field also, which will do. But this is the major thing to know that this is the Ising Hamiltonian. This is the general Hamiltonian value for any dimension. You can have two dimensions.

You can again have spin up and down exactly same thing. This is called lattice; they are number of nearest neighbour. Here it is 2, it becomes 4. If you go to triangular lattice, then number of nearest neighbour becomes 6, then you can go to fcc or bcc lattices. That is just a historical comic that when you go to three dimension you cannot solve it analytically and you fall back on a high temperature expansion, which is very similar to Mayer's.

It is really interesting and huge number of people during 60s and 70s used to do these high-temperature expansions of the three dimensional Ising spin, very famous scientists; nobody did it. So we have now defined the Ising Hamiltonian and now I spend a little time telling you why such a simple Hamiltonian, it might not look so simple to you, because if you are not used to kind of abstract things.

This is sum over i and this is sum of given one configuration. So I have 1 2, 1 3 and 2 3 just like we did Mayer’s theory. So this Ising Hamiltonian, I now spend a little time before I go to calculations to tell you, what are the basic merits and certain things of this. You know what a have in notes is much better than written but it is better than that. But let us see this will do little bit of the work, that i intent to do. There are too much detail here.

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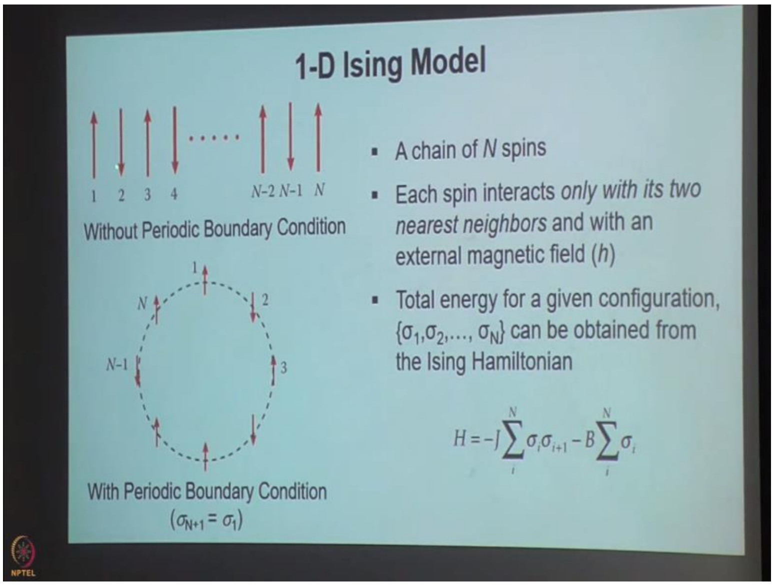

So they are lattice models. So some of them analytical solution as possible. So this is this spin that I am talking. A chain of N spins and this is the Ising Hamiltonian and you can understand now, what is important thing to realize, they are N spin. Now at any given instant or any given configuration, these spins are all having configuration which is different from another configuration but each configuration comes with an energy.

So a given configuration this Hamiltonian is for a given configuration. For example, let me consider this one. I will pick up a minus from here. Let us say magnetic field is 0. I do not need it now. I will not need it for some time. Now I will pick up a positive contribution from here another positive, another positive spin, here is positive. We will do it is all anti ferromagnetic kind of interaction.

But if each were up, then this thing, so a given configuration comes with a given energy, which is the exactly same we have in gas phase that where at any given configuration N number of particles are interacting with each other and that configuration has an energy. And Boltzmann taught us that the weight of that configuration will be given by the energy of that configuration and this is very essence of this statistical mechanics. How we will be thinking in statistical mechanics.

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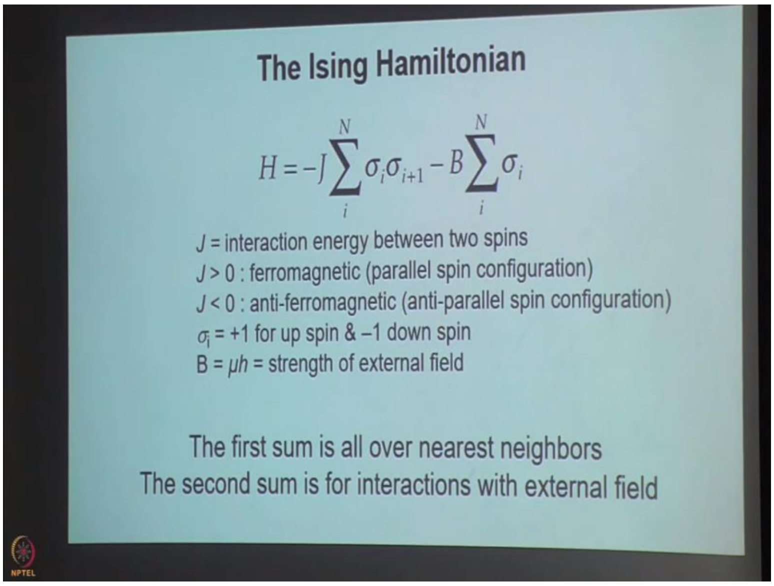

So again the Hamiltonian given,

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

here one says what is ferromagnetic, what is anti ferromagnetic, all these things. Now how do I do the partition function?

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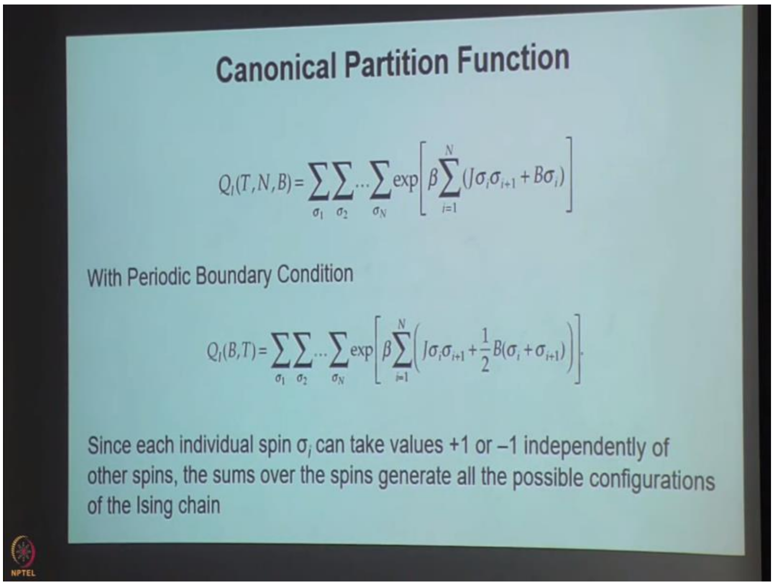

Now in partition function, these Hamiltonian has to go in the numerator of the exponential, minus is there in front of $-\beta H$. That minus takes care of the minus and minus here I get positive. Now the difference between my earlier thing is that I have to add over all the configurations. So before the sum over spins goes here in the exponential, but this is weight of a given configuration, but I have to sum over all possible configurations.

So this is the same as in my classical or continuum statistical mechanics. The integrations over positions is the same as the sum over spins. There I take a configuration, particles are in the position R1, R2, R3, R4, RN and then I get a Hamiltonian for that. Then what I do? I integrate over all possible positions of the first particle, second particle, third particle, dR1, dR2 … dRN, which is exactly same thing we are doing here we are summing over all possible spins.

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

With periodic boundaries

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

But now you understand that it creates enormous number of configurations, because these spins though only can be up and down, it has N number of spins are there, they 2 to the power N and if N is large number like Avogadro number, then you have a huge number of configurations there. So the entropic part enters through all possible combinations and the Hamiltonian comes. so now the partition function is this thing.

This we need not worry right now.

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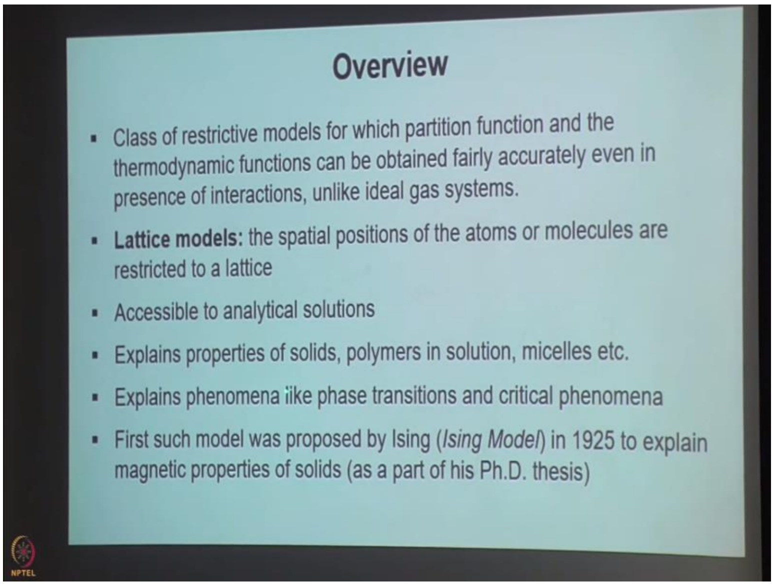

So now I want to the go back. So this is particularly for Ising model, solids, and polymers micelles, reverse micelles this simple thing is used rather extensively. And also the Ising model that we do is used for gas liquid transition even condensation. You can have a nearest theory version of the Ising model or Ising model version of the Mayer's theory and this is the one most part of this.

Now what I am going to do? I am not going to do this difficult thing. I will do something a little simpler and because it would become very difficult. So I think I have explained that these particulars spin comes with an energy. That energy goes to Boltzmann factor in exponential and that gives the contribution to partition function of this particular configuration. This is not good. That is the one we discarded right, yeah.

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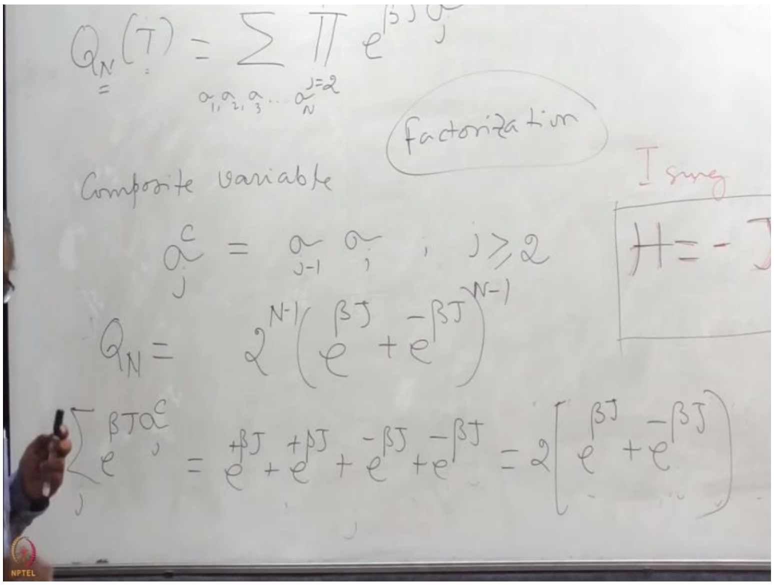

Now I am going to consider only this part. I am neglecting for simplicity now, because I will be able to do something. So I now have a partition function. QN to the function of T, N number of spins at the temperature T, σ 1, σ 2, σ 3, all the spins, then e to the power – beta BJ/σ 1 σ 2 + σ 2 σ 3.

$$Q_N(T) = \sum_{\sigma_1,\sigma_2 \ldots \sigma_N} \exp\left[\beta J\left(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \ldots + \sigma_{N-1}\sigma_N\right)\right]$$

So this is the partition function I need to evaluate with the condition that σ 1 σ 2 or they can take up and down.

Yes, it should be plus. So now you notice the one thing that all these are coming as product. So I can introduce a composite variable σ_j^c

$$\sigma_j^c = \sigma_{j-1}\sigma_j$$

Now let me see what are these composite variables we take? Now composite variables will be when this is plus, this is plus, then minus minus, again plus. It is a plus-minus, minus.

So composite variable, when each of them have two variables, composite variable has four values. So these quantity now I can now write in terms of composite variables which is

$$Q_N(T) = \sum_{\sigma_j^c} \prod_{j=2}^{N} \exp\left[\beta J \sigma_j^c\right]$$

Now I can now calculate these contribution of these, of course I have to do j greater than equal to 2, because I have 1 2, 2 3 like that. So j goes from 2. So in this case j has to go from 2 to particle N. Now I have to do this composite variable.

So now I write this as, I bring the product outside and I take this sum inside.

$$Q_N(T) = \prod_{j=2}^{N} \sum_{\sigma_j^c} \exp\left[\beta J \sigma_j^c\right]$$

So now that will be e to the power beta j σ composite variable c and sum over say jz spin, then σ_j^c has 4 values. So that will be

$$\sum_{\sigma_j^c} \exp\left[\beta J \sigma_j^c\right] = 2\left[e^{-\beta J} + e^{+\beta J}\right]$$

I have plus minus e to the power minus minus plus plus both minus. Then a plus minus and minus plus. So that would now be 2 into e to the power beta j, beginning to take the character of Ising model. So what I have done actually is equivalent to a factorization. I have factorized. I could factorize because of this form of, what I delineate the form of that thing. So I have done a factorization, just the factorization I do.

But that factorization suddenly gave me a wonderful form which now does not depend on j, that is the beauty. Then what I can do now? I can make this product here. So now I can replace now this by, so many times the product e to the power N, N – 1 but N is very large. So I do not really care of that.

$$Q_N(T) = 2^{N-1}\left[e^{-\beta J} + e^{+\beta J}\right]^{N-1}$$

So I have evaluated the partition function in the absence of a field of the Ising model. Let me do some work with that way.

The way I always did was like these. This is the way I always decomposed factorize. That is the way I learn, but in the book that we have written is not like that and that is this lacuna, we have to really correct because this is the way one should go. But most of the books jump into, probably Kerson Huang has this way of doing things because I remember that this is in many places the composing variable.

But unfortunately most of the places I looked into they start with a very complicated transfer matrix, all these things which is at least what you can ask for physical chemistry by known people is not a best way to start these things.

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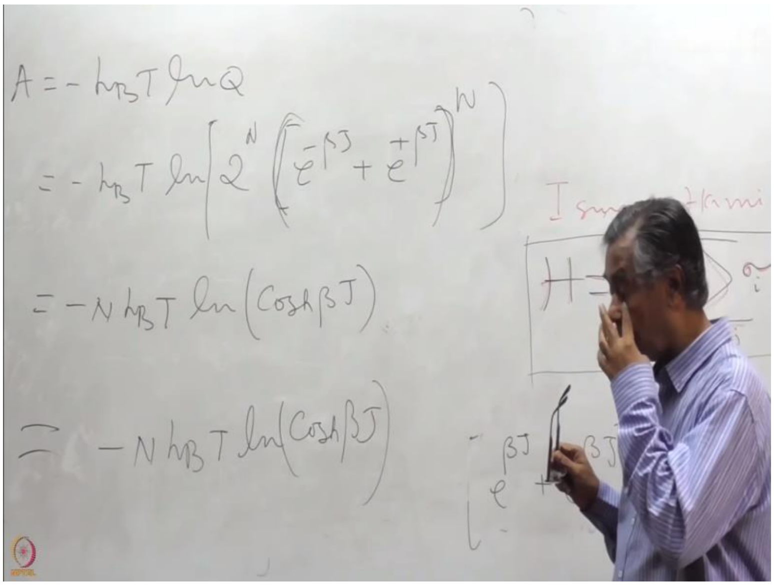

Now there is some extremely important thing coming out from there.

$$A = -k_B T \ln Q$$

Now free energy A, that is then I am just neglecting N is very large. So I am putting that equal to N. I am doing on this right.

$$A = -k_B T \ln \left\{ 2^N \left[e^{-\beta J} + e^{+\beta J} \right]^N \right\}$$

What is this quantity, again 2^N, then $k_B T$. So RlN here, so this term I want to take it out. So + 2n KBTl into, please tell me if i did anything wrong. So these two cancels, so I am left with partition function, the free energy.

$$A = -Nk_B T \ln\left(\cosh \beta J\right)$$

So in the absence of a magnetic field, I have obtained the free energy. I have obtained the partition function and the free energy. Now there is something very important here, you may know. This continues to be in presence of a magnetic field. The important part here is that there are certain functions in mathematics, which are called entire functions. Exponential is an entire function. Cosh is an entire function.

What is an entire function that has infinite number of derivatives and is continuous all through. That function is called an entire function. So this cosh is an entire function. So it cannot show any discontinuity. If it does not show any discontinuity, it cannot show any phase transition, and one of the primary result of the theory of phase transition is that you cannot have a phase transition in one dimension.

So this is a also called a beautiful theorem as Ashcroft-Mermin theorem, but we do not need to go Ashcroft-Mermin theorem at all, atleast not in this kind of rather preliminary things that we are doing. But it is important to know that these cannot show any similarities. So it cannot describe phase transition. I can calculate entropy. I can get dA/dT on that and get the entropy. I can get this specific heat and then I can calculate the fluctuation in energy, the specific heat.

And then I can find those two are the same. All these things one can do and people have done because this is the one model which has been waiting today. But important result here is that because of these kind of beautiful expression, nice neat analytical expression that we do have completely analytical function. So there was this, this gave rise to a lot of logic and a lot of controversy that a little bit of history that how statistical mechanics can at all describe phase transition.

That means since Boltzmann is exponential and exponential is an entire function, if differentiable completely to all order how come then is statistical mechanics which is in the form of the sum of the exponentials, as we have seen here, sum of the exponentials can give rise to a singularity. That was a huge debate for more than 2 -3 decades which was ultimately solved in a specific case by Onsager.

But in a very general case a beautiful by C. N. Yang and T. D. Lee called Yang-Lee theory or Lee-Yang theory, two very famous physicist who also did quark and parity violation and they went on to get the Nobel Prize for that, but there another beautiful work was showing how and they used the Ising model and used the Mayer’s theory, actually more Mayer’s theory than Ising model to show that how singularity can evolve by doing a beautiful piece of complex analysis that we can do sometime. So this is in the absence of a magnetic field.

In the presence of the magnetic field, it is a little bit difficult. So I will not do it in the class but I will go through that little bit and then I will give you the final result. It is not too important that we do it for the major way course of the thing. Those of you who are interested, you can do it and if you get stuck, you can come to me and I will do it.