Basic Statistical Mechanics
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Lecture - 47
Ising Model and Other Lattice Models (Part 4)

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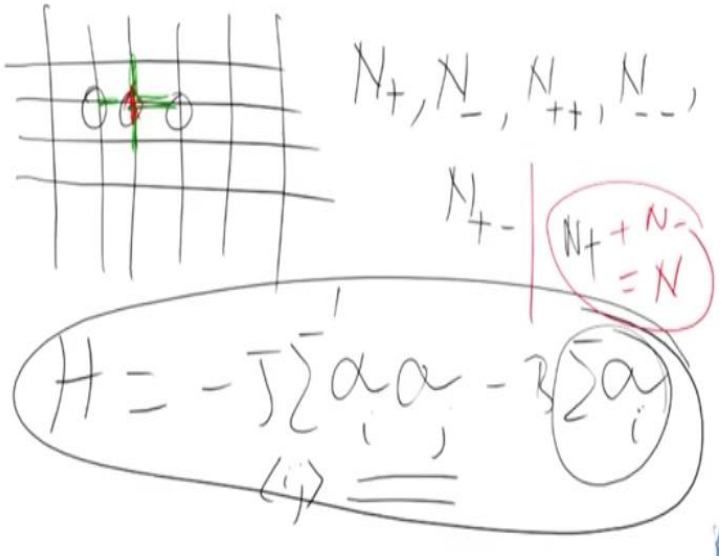

I start doing the nearest neighbour interactions. So I consider again a lattice and I will tell you where I make the mean field approximation. To a great extent, you will see the things will be done exactly. To a great thing, it will be done exactly, then at some level, we will see a very intuitive approximation will be there. So in order to get started, let us see the following things. Since we are talking of nearest neighbour interactions, I have the following variables.

So at a given configuration, so if I want to write the Hamiltonian, so let me write the Hamiltonian again H as $-J\sum_{\langle ij\rangle}\sigma_i\sigma_j - B\sum\sigma_i$, i, j are nearest neighbours. Then I have –B σ_i .

Now look at this, so what does this term depends on. This is the nearest neighbours. It depends on whether they spin up, how many of my spins are parallel, how many of my spins are anti-parallel. So now I introduce the following things, number of spins, which are up and down is here.

So I have number of spins up, one variable N_+. I have number of spins down, one variable N_-. I have number of nearest neighbours, which are up, because that comes naturally here N++. Then I have number of spins, which are down, parallel, then I have which are plus and minus, one parallel and one anti-parallel. That means, in this Hamiltonian, I have 5 variables. These can be expressed in terms of these 5 numbers.

However, one thing we need to now know and this is something you should wonder about and there is a relation between N+ and N-, that means N+ + N- = N, right. So there is one condition, so I don't have all 5 independent variables. I have right now 4 independent variables. Then, there is a very interesting thing, which is that if I take all the spins up, I just ignored all the negative spins right now. I take all the spins up and then I draw a line between.

From the up spin, I draw a line, let me draw that in green line. I draw a line to the nearest neighbour. So I pick up only the up spins and from the up spins, I draw a line to the nearest neighbour, because I only have nearest neighbour interactions. Now this is something very nice. So if my these spins are also up, then I draw one from this, then I draw another from this. So in this case, what we will have, a double line between.

I will have a double line between two up spins, but if it is a down spin, then I will have one line. So to begin with, let me summarize. I pick only the up spins and from the up spins, I draw a line to the nearest neighbour. How many lines I will have? I have gamma nearest neighbours and from each up spins, I am drawing to the neighbour one.

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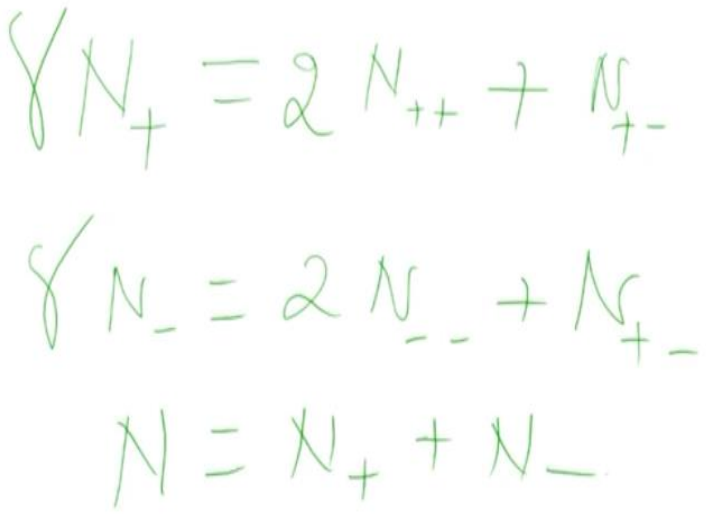

Then I will have gamma N+. That is the total number of lines that I draw. What then it will be equal to, there will be N++ will come with 2. So this is the conservation condition that must be obeyed. In addition, with N = N+ + N-, which is a conservation condition, I get a second conservation condition. Now, I say, okay, I want to do the same thing, now starting only with the down spins. Again I get this relation. So what do I get now?

I get three relations. So I start it with 5 variables that comes into that interests the Hamiltonian, but now I find that those 5 variables are not independent. They have three relations between them. So I now have essentially two independent variables. Now that now tells me, okay, if I have a choice that I can have two independent variables.

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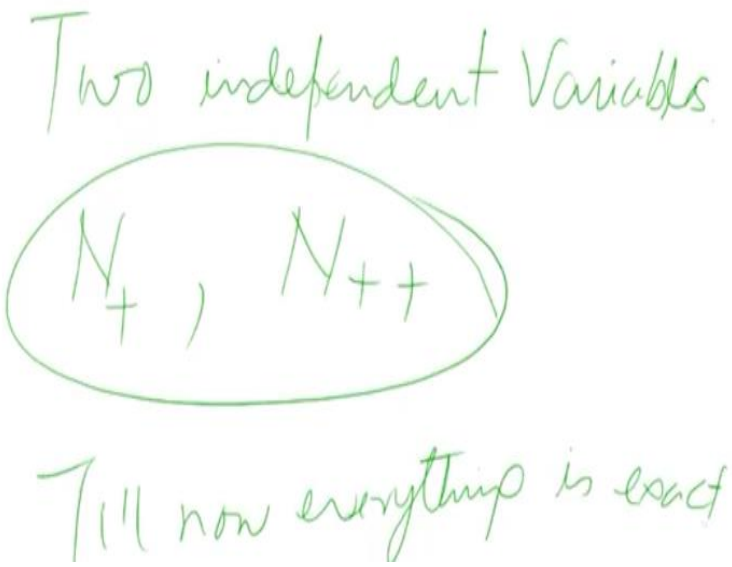

So what are the two independent variables, I choose. Can you make a guess? One of them, I will make either N+ or N-, but only one of them is possible, so I take N+. Other I take N++. So these are now my independent variables. Everything else has to be, so I have to now express N+ and N++ in terms of all other things. So I can eliminate all those other variables and I will express N+-, N-- and N- in terms of N, my total number of spins and these two.

So once I can do that, I can now write the Hamiltonian in terms of only these two variables. Still now, everything is exact. So we will go very far by being exact, then we will make a very significant contribution and that is the significant assumption, which is the reason that I want to do this mean field approximation in a very robust and systematic way, because this is something with majority of the students, at some stage, just like Landau theory, will use in and out.

Similarly, this is the very general way of doing the things, which finds lot of applications in the future research. So we now with me, bear with me for a minute. Now we have the relations and we now need to eliminate and get. So we have done that. Now I do, go back to Hamiltonian. There is large number of steps involved. Even the mean field theory calculation is fairly nontrivial. Any Landau type theory is highly intuitive and not technically nontrivial.

Van Der Waals is not nontrivial, but those do not have the details of interactions. So when you want to build in the details of intermolecular interactions, like here we are doing spin-spin

interactions and you already have the experience of Mayer's theory, which was of course not mean field. Things are not easy. So one has to do, I remember one class I was taking at brown and I have a small story to tell you that and we had the great, great Leo Kadanoff was teaching statistical mechanics.

I was fortunate to have his class twice, one at brown and one in Chicago. Now Leo Kadanoff was really doing these very difficult problems and in his course. So there was a post-doc or student I do not remember from Noble Laureate Leon Cooper, and who was you know pretty good. So one day Kadanoff asked now what is your opinion, with students in general on how the course is going or how do find it? That is the way actually people go.

They always ask that at some stage that how are the things going and this student, whose name I forgot then told Leo Kadanoff that his grades are nice, but your problems are not elegant. Your problems are too laborious and elaborate and boring. So it is not elegant. So Leo Kadanoff got very upset. Then Leo Kadanoff went on saying (()) (10:20), he made long lecture and the summary of that was the following: He said that look in physics it is 90% of the time or 95% of the time, you just do the hard work and you have no chance of being elegant.

You are very lucky 5% of the time you get to be elegant. So better you know that doing theoretical physics or any theoretical science is huge amount with hard work. But you do that hard work, because you like this kind of a work, but do not expect that you will get the chance of being elegant. So we will see now, a large number of steps that we do and we will go back and forth and to make it easy for the students, I will give a flow chart and go through the flow chart and then do that.

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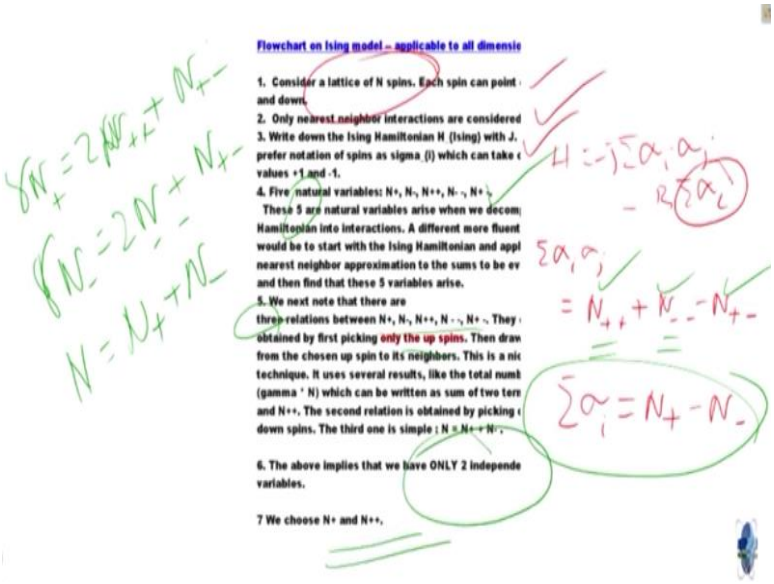

This is the way, I hope you can read, but I will read it for you, if not, because I do not think it is very big, but this will passed on to you. There are certain problems on the right side that would be then corrected in the notes that you will be handed over with the course. That means, you will be able to read it here anyway, but you will be seeing that final thing more complete. So we consider lattice of N spins as I said.

Only nearest neighbour interactions, right down Ising spin Hamiltonian H. So this H I write down in terms of $H = -J\sum\sigma_i\sigma_j - B\sum\sigma_i$. Now if I write down, down then this following thing, $J\sum\sigma_i\sigma_j$ gives me, $\sum\sigma_i\sigma_j$ with nearest neighbour, I get the following results. Please check it out $N_{++} + N_{--} - N_{+-}$. Now I can do $\sum\sigma_i = N_+ - N_-$. That is because plus spins comes with +1, up spins top spins come with +1 with those pointing towards up, they get +1, those are -1.

So that is this thing. This is this thing and then $\sigma_i\sigma_j$ is then plus-minus, so when they both are plus, say both are minus, as I said before. So then, then you see this 5 variables are coming, 1, 2, 3, 4, 5. So 5 variables comes just from the Hamiltonian. We are not introducing them, just like that, it is the necessity of the calculation. Every step that I am going to do is very logical and they go from one step to another step and systematically.

The beauty of this thing that I am doing, why I am not doing the 2D Ising model and doing this thing is because this gives you piece by piece, minute by minute more value for your time than the other things. Now then, there these 5 natural variables come. Note that they are obtained by picking. So there is a relation. There are three relations as I said, when we have done that between them. They are obtained by picking first only the up spins and in the up spins then you write down that what are the up spins and the condition we remember $\gamma N_+ = 2N_{++} + N_{+-}$. Then $\gamma N_- = 2N_{--} + N_{+-}$ and of course we have the other condition $N = N_+ + N_-$. There we have only 2 independent variables and we choose, as I said, N and N + 1. Now we continue with these things.

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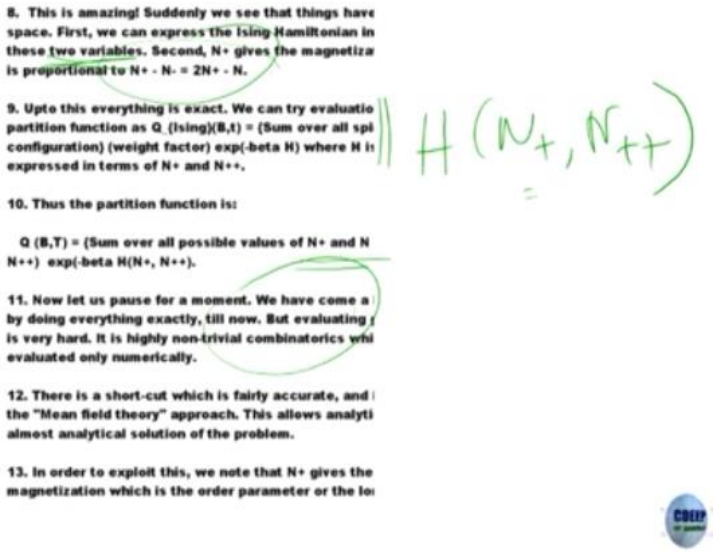

This is amazing. Suddenly, we see that things have become very simple. We can express the Ising Hamiltonian in terms of these 2 variables only and so these proportion are 2N+ and N-. Up to this point, everything is exact. Now we will go on till now for quite some time, which will be exact. So I go back to partition function, sum over all possible values of N_+ and N_{++} and then I write the Hamiltonian now in terms of N+ and N++.

Well, I have not written down for you, what would be that I will do in a minute, what will be the real Hamiltonian in terms of N+ and N++, that I will do in a minute, because I have to eliminate those things, which are little time consuming. As I said, we have done everything exactly and now after one does the shortcut using the mean field theory.

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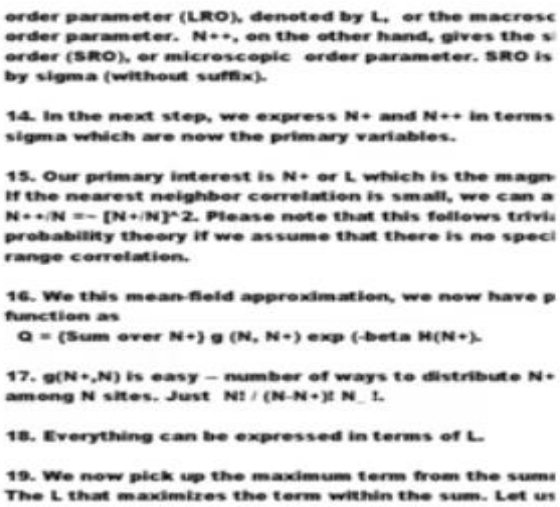

Now before I go to mean field theory, I just want to draw this thing that why I need the mean field theory. So at this point, it turns out with these everything is exact up to this point and here we get stuck, because we cannot evaluate the partition function with N+, N++. This is the main problem two dimensional Ising model, three dimensional everywhere, but this is where we will be able to make an approximation, very enlightened approximation.

So now I am going to go and do a little bit more calculations and go a little bit further and let you know. So I have now used this, I have to have these three relations. I can now show by using these three relations.

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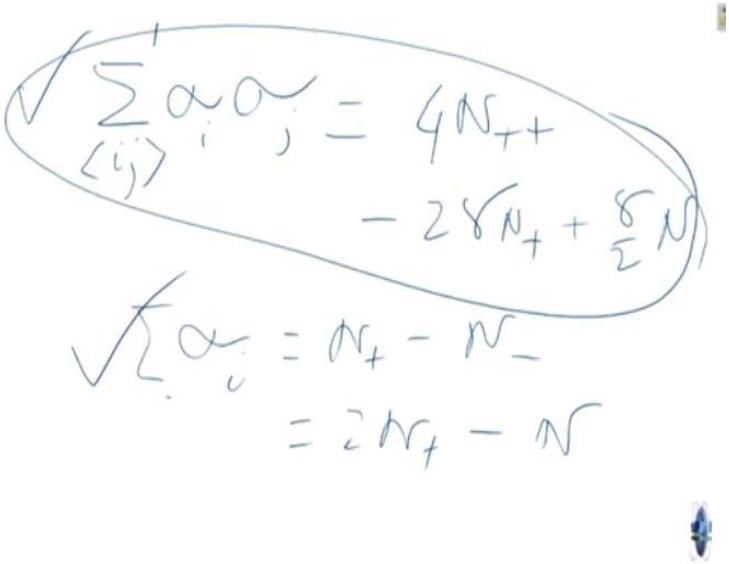

This you can verify. Everything only in terms of N+ and N++ and $\sum \sigma_i = N_+ - N_-$. This is alright, so I have, this is the one trivial. This one I get by substituting into N++, then I have N-- - N+- that is this thing. Then I eliminate N-- and N+- in terms of N+ and N ++. When I do that, then I get this equation, just a trivial exercise, all of you can do that and then this one and I have j in front. So I now have the Hamiltonian in terms of N+, so I now go, I said okay.

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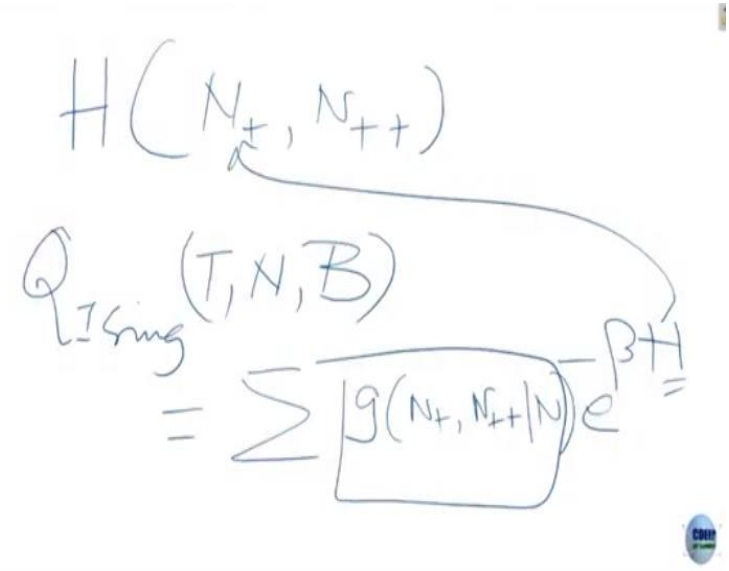

I have the Hamiltonian H as a function N+ and N++. I have the Hamiltonian. So now what I need to do? I have to write the partition function of Ising as a function of T, temperature, total number of spins N and magnetic filed B. What do I need to do? I need to do g, this H. If I can do that, I

am all set, but I can express H in terms of N and N+, but I cannot evaluate this quantity. This is now the final barrier that we faced. Till now, everything is done exactly, but you cannot do that. So we are stuck. So let me write down. I have already written down the Hamiltonian, but by combining those things, still I can give you once more.

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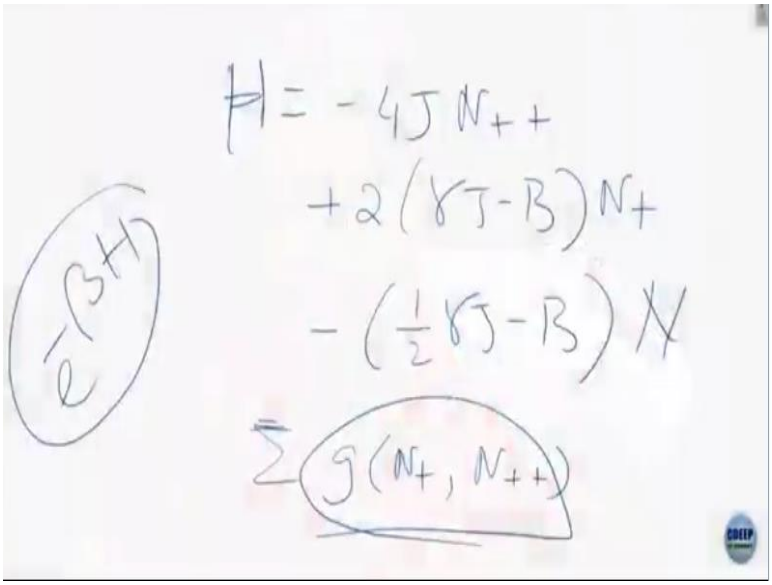

The total Hamiltonian H = same I am doing $-4JN_{++} + 2(\gamma J - B)N_{+} - \left(\frac{1}{2}\gamma J - B\right)N$. So this is the Hamiltonian. So $e^{-\beta H}$ that has to go, this H of course goes there, but in front this part is okay, but I need to evaluate g. If I could evaluate g, the number of ways I can find out N+, I will give you N and N+ and if you can give me the number of ways you can realize that configuration with the given N + N + - 1, then if I can give you an expression, then I will be able to play the trick that maximize the partition function and minimize the free energy and pick up the term, but I do not have any clue to that. Now how do you do that? Now I will go one step backward and I will do something really very, very interesting. So now I introduce two terms.

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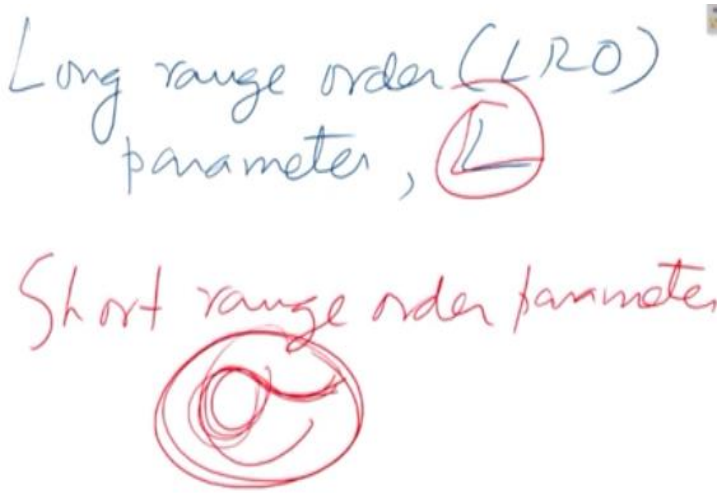

One is called long range order parameter L, another is short range order parameter. Now I introduce, remember L long range and, sorry, I will change the notation. I will again call it σ, but without a subscript. So short range order parameter sigma for S. This is universal notation, so I am going. In many books in order to separate, they say instead of σ_i, σ_j for the up +1 and -1 values of the spin, up and down they use a Si and Sj, but σ_i, σ_j is the more common thing and short range order parameter σ is also fairly common, but since we do not have any subscript or superscript to sigma, we will have no problem, that means short range and long range order. L for long range, sigma for short range, this is easy to remember.

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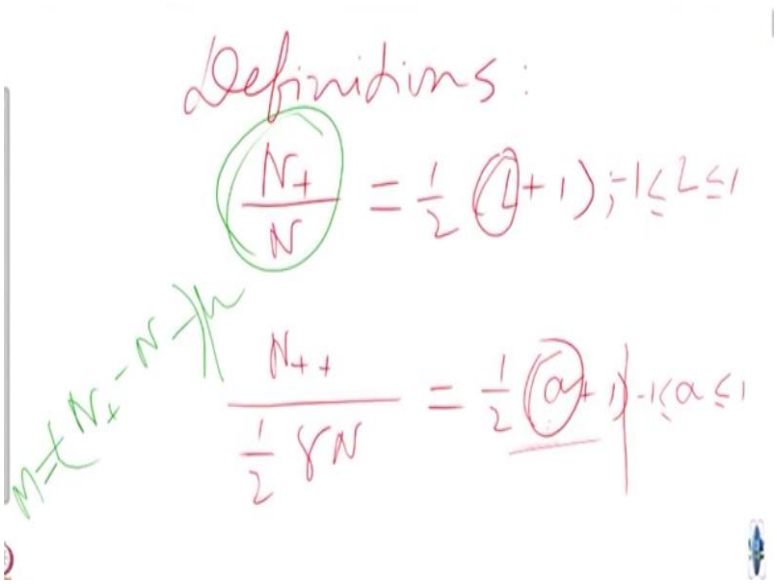

So now I define in the following way. Definitions, very nice definitions the fraction of up spins and double spins, so L clearly you can see, $(-1 \leq L \leq +1)$ $(-1 \leq \sigma \leq +1)$. So when L is 1, then this is 1 + 1 2 and these 2 gets into 1. That means all the spins are up. So in long range order parameter is 1 means all the spins are up, system is fully ferromagnetic. Short range on the other hand is the following way.

Again σ is 1 and this is half γN. γ N is the number of nearest neighbours, so in order to avoid double counting, you put the half in front of it, because you have N++, you can count this on the same way, so half gamma N for that. Now σ is 1. When sigma is 1, then it becomes that is N++ becomes equal to half γN and then on the other hand if that is all the short range parameters are up, all nearest neighbours are up and on the other hand, when it is -1, then this is 0, then you do not have any up spins, everything surrounding, your nearest neighbours all spins are down. So these are the definitions of the short range and long range. This is long range. Now look at this long range order parameter. It is very, very intuitive and very interesting. This is nothing but, as I told you, total number of spins. This is nothing but, when all the spins are up, I know N+, I know N, then I know N- and N+ - N- is nothing but the magnetization M.

That is the magnetization. So if I know N+, I have the magnetization, the problem I want to solve. N++ on the other hand is a microscopic quantity and I do not have any handle on that, except I know when many, many spins are up. When there is a ferromagnetic state, not all spins are up. It will be a ferromagnetic state, all you have to do N+ is greater than N- and you want that ferromagnetic state to be established or a significant number of spin greater than that, by a phase transition that means, it has to jump from low magnetic state to high magnetic state, that happens at certain temperature. So it is the essential part of change of magnetization in a singular way. Now I want to capture that part, but I do not have, as I said much of a handle of N++, except that when in a magnetic state, then N++ would be more than N+- and more than N- -, because there are more spins that would be up. Other than that, I do not have any handle on that.

Of course, I know if ferromagnetic interaction is low temperature, there are more up spins. So this is the situation that we are now dealt with. So we have done till now, all the things correctly, but now we are going towards something physically inside, because we have gone as per as we

can, exactly by decomposing into N+ and N++, eliminating other things, everything is exact. Gamma changes in two dimension. Triangular lattice is 6. Square lattice is 4.

Then, in three dimensional lattice, cubic lattice is 6, bcc is 8 and fcc are 12. So we know that and so the only thing that is taking care because of the nearest neighbour interactions is γ, on tuning gamma I am capturing the power solid system, but we have gone as far as we can, because we cannot evaluate the number of state, gN and gN+ and N++. So now long range and short range order parameter has two physical changes. Can you work with that? And that is what mean field theory does; they work with this. So now I want to express the next following thing. I can now go, since N+ and N+- are again in terms of.

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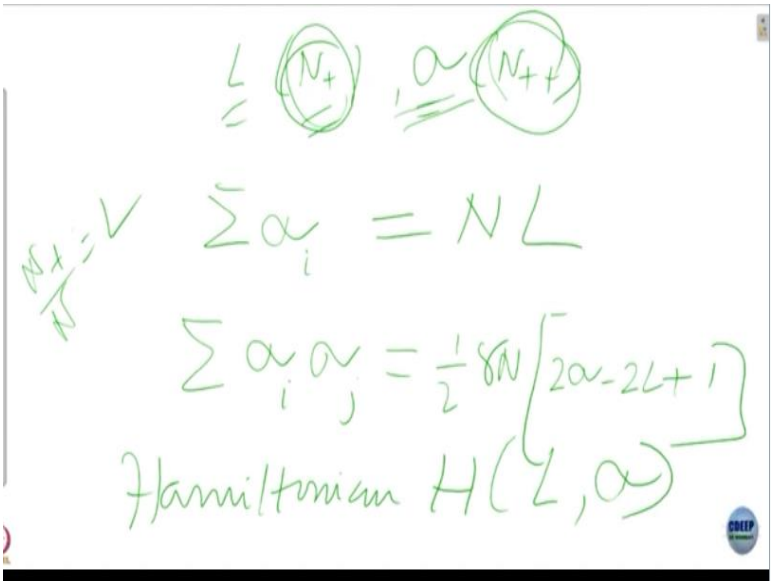

So L is in terms of N+, N++. That immediately tells you now I will be able to write the Hamiltonian in terms of L and sigma. So in the state of a microscopic kind of theory, this is not microscopic, this is microscopic. I am going to go into order parameter and then I can hope to make an assumption and approximation. So let me write down the Hamiltonian in terms of L and sigma. So I can write this thing like that, $\sigma_i . \sigma_i$ is very easy to say.

It is NL, because N+ by N and now I can also write. I can show that this you can do, because we have done σ_i, σ_j before, few slides before, we have evaluated that. Now I just put the definition of L and sigma and I get the following thing. I am just writing it down. So I can now write the

Hamiltonian, so I write the Hamiltonian H in terms of L and σ . Now what do I do? So what I do now is make an approximation.

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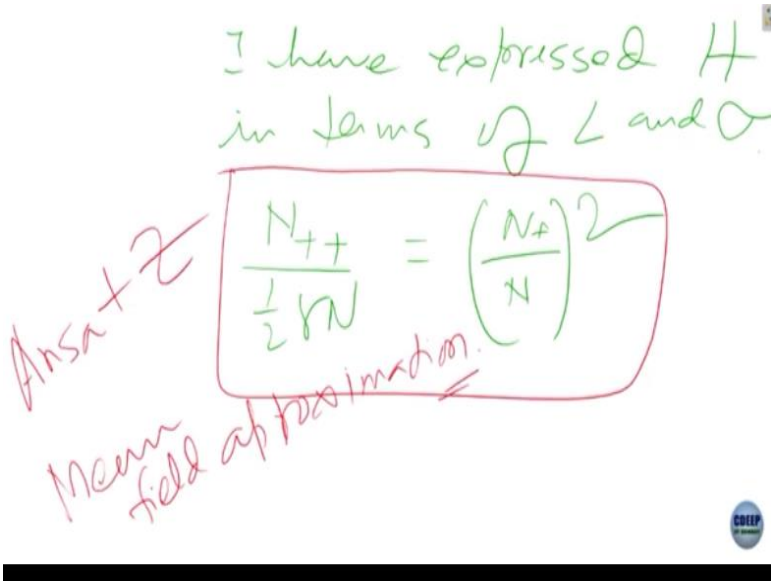

So I have expressed Hamiltonian. I have expressed H in terms of L and sigma. So I have introduced two qualitatively nice things, but I have really not made any significant progress other than that, but now I look one thing. Now I am going to make an approximation. Now I say the following things. I go back to probability and I say, okay, my probability of having two consecutive spins up next to each other, nearest neighbour.

If I now assume that this probability that it is up, is there independent of each other. So there are multiple application of this being up. Then, probability of pN++, so the fraction of N++ would be same as $\left(\frac{N_+}{N}\right)^2$. Now make the approximation, the fraction of N++ of the possibility is this. So this is my answer. This is my mean field approximation. That means, there is no short range order other than what is contained in long range order.

So this is the essence of mean field approximation that you ignore the short range correlations and you say short range correlation is given by the long range correlation. So once I make this approximation, what do I achieve after this approximation?

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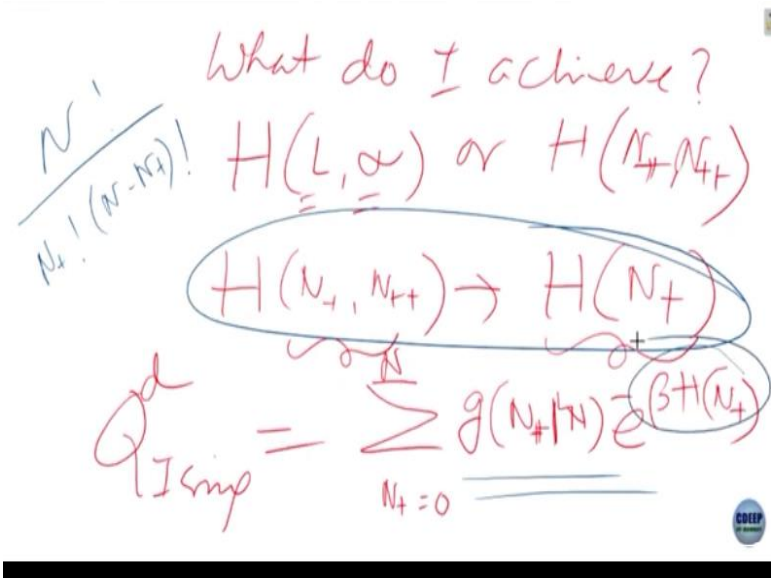

What do I achieve? I have now eliminated. So I do that, I already have in terms of L, sigma or N+, N++. I am going to L and sigma to get the physical essence, long range and short range order and I say short range order is those same from long range order. Probabilistically, I can argue that N++ is given by N+. So I then eliminated by one logic, one more variable. So I have eliminated the N++ by leaving that condition.

And once I eliminated N++ what I do? I go back, I already have H in terms of N+ and N++ and I get that now H in terms of N+ only. I have the Hamiltonian in terms of these two now having terms of that. Then, what do I gain after making the approximation? Now, if I have this Hamiltonian in plus, my Ising model partition function for any dimension d, sum over all N+ that can be from 0 to N number of states I can distribute N out of N spins and how many ways I can get N+ out of N, beta Z +.

So what is the whole cracks of the thing, is this reduction and once I can do, I write this is approximate. Of course, this is approximate, is an answer, but I can now write this, but lo and behold, I know that, that is nothing but N! by N and I know this quantity. So now I can go from this sum under the summation, I can find out the maximum terms. So at the end of this long road, we are in a position now to exactly evaluate the partition function, exactly related to energy.

We will take a short break now and we will come and do that by following the most elegant description that I know half of this problem, that is Kerson Huang (34:40) one, but basically what I say I will probably we will first evaluate that and take it to the results.