Statistical Mechanics
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Lecture - 24
Examples of Microcanonical Ensemble - Magnetic System and Ideal Gas - Part 1

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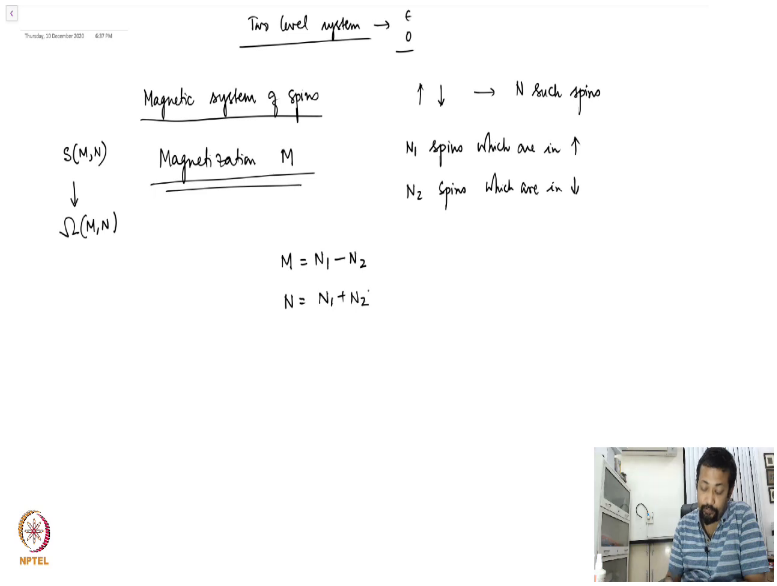

So, now that we have looked at the very simple two-level system which can exist in the energy levels 0 and epsilon. Let us look at something a little bit more complicated. It is still a two-level system, but it is clearly, it has a experimental relevance. What we want to look at is a magnetic system of spins and this we have discussed earlier also.

So, the spins can be either in a up or a down state and there are N such spins right. Now, this magnetic system has a magnetization M right. So, if there are N 1 spins which are in the up state and N 2 spins which are in down state correct; further, we also have to look at this condition, where my total magnetization is given.

So, essentially, what I am trying to find out is S as a function of M comma N and for these, I have to figure out the configurations which are possible M comma N. Not just N, but given a value of magnetization and the magnetization M is N 1 minus N 2; number of up spins minus number of down spins and N is N 1 plus N 2.

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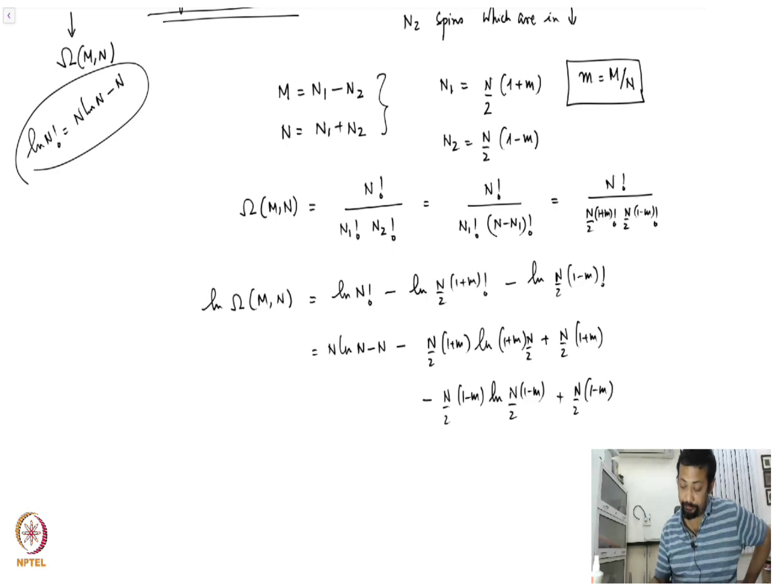

So, this actually simplifies our life one can use these two equations to write down N 1 is N, 1 plus m by 2 and N 2 is N by 2, 1 minus small m; where, I have defined the small m. This is now no longer an extensive quantity, but this is a magnetization per spin.

Now, it is purely a combinatorics. If I want to find out S as a function of omega; S as a function of M comma N, I calculate the total number of microstates and that number of microstates is given by N 1 factorial N 2 factorial right, which would mean that this is going to be N factorial N 1 factorial N minus N 1 factorial correct.

So, now, we will keep it as N 2 because we have already derived an expression for N 2. Omega comma N is now it is a long algebraic process. So, this we will write down as N factorial N into 1 plus m by 2 factorial N into 1 minus m by 2 factorial. So, this is ln N factorial minus N into 1 plus this factorial minus ln N by 2, 1 minus m factorial.

We use Sterling's approximation which tells me that ln N factorial is N ln N minus N. So, this becomes N ln N minus N, N by 2 1 plus m ln 1 plus plus N by 2, 1 plus m minus N by 2 ln. Sorry. So, ln N 1 minus m by 2 plus N by 2 ln, no this is just going to be 1 minus m.

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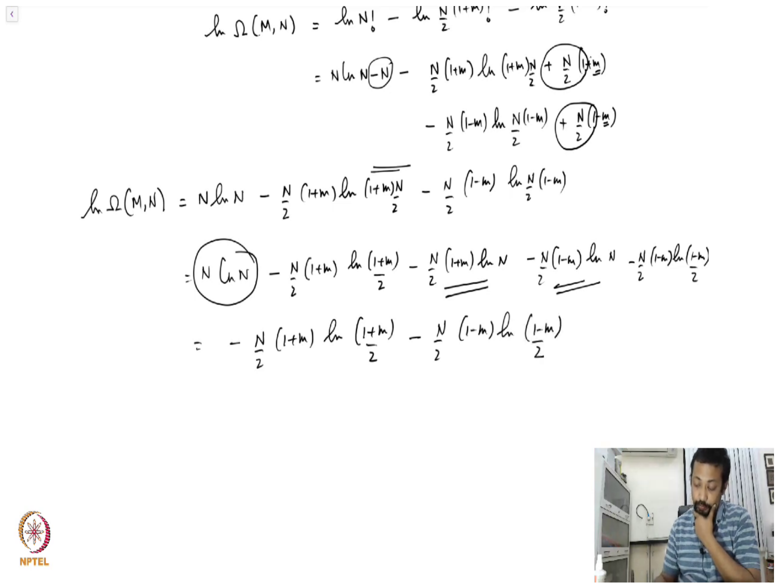

So, ln omega M comma N is equal to again one has to go through all these elaborate things, but some of them are pretty easy to figure out right. So, you see this minus N is going to cancel out with plus N by 2 and plus N by 2 from here right. So, essentially, you will have and this is going to cancel out because they do have opposite sides. So, you are going to have N ln N N by 2 1 plus m ln 1 plus m N by 2 minus N 1 minus m ln N by 2 1 minus m right. Good, so N ln N N by 2 1 plus m ln 1 plus m by 2 minus.

So, we are expanding this part here minus N by 2 1 plus m ln N minus N by 2 1 minus m ln N by 2 minus N by 2 1 minus N ln 1 minus m by 2. Sorry, we will not include the 2 over here. This means that if I take this expression and if I take this expression, I am going to get minus of N ln N. So, N by 2 1 plus, I am left out with this nice little expression minus N by 2 1 minus m ln 1 minus m by 2 right.

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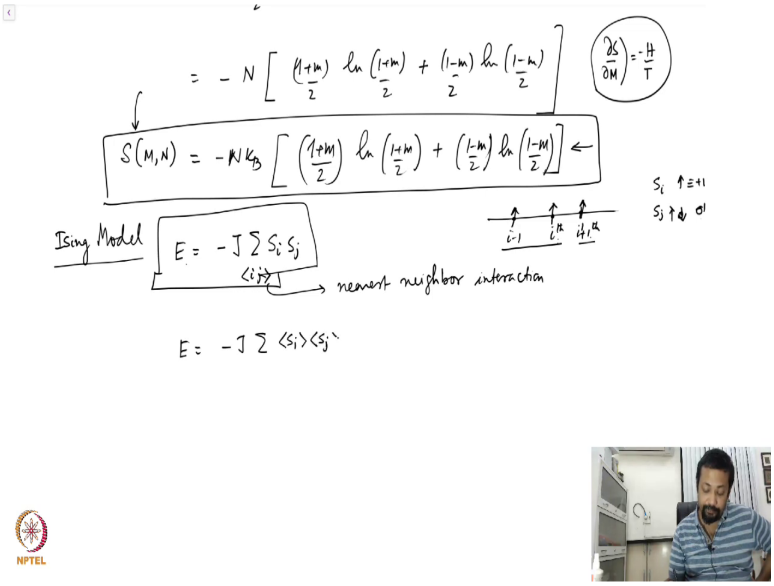

So, I can take N outside. This tells me it is 1 by 1 plus m by 2 plus 1 minus m ln 1 minus m by 2. And therefore, the entropy S comma M comma N is minus NK B 1 plus m by 2 ln 1 plus m by 2 plus 1 minus m by 2 ln 1 minus m by 2. From this of course, one can calculate del S del M and this is going to be H over T; the magnetic field.

This is going to be one of the equation of states. Now, clearly, what we see over here is that this entropy does not has no energy over here because when we started off, we said that we have just N spins and this spins can flip without. So, there is we did not even specify any interactions so, just that the spins can fit independent of each other.

Now, I want to specify that the flipping of the spins is dictated by the interactions. So, let us say I write down that the energy is minus J sum over Si Sj right. So, this means that if the ith spin and this interaction i and j can happen only over the nearest neighbor.

This angular bracket indicates nearest neighbor interaction. So, which means that if I have a lattice, I have the ith spin, I have the i plus 1th and I have the i minus 1. So, if this spin is up, then it tries to flip this spin towards itself. The interactions are only between i and i i plus 1 and i and i minus 1.

Of course, this model in physics is very simple model of magnetization and it is called Ising model. We will not study it here, but we merely want to exploit this only in what is called mean field limit. Look good.

So, let us say I have now there is one more thing that one has to look at is that this particular expression does not care about the dimension of the space right. I have never said that this spins are sitting on a one dimensional lattice. It can spin very well, spin sit on a three-dimensional lattice; but this is purely pure entropy; good.

So, this is this entropy is purely due to your configurations of the spins. Now, I bring in the internal energy right. So, when I bring in the internal energy, I said look, you have to there is an interaction between the nearest neighbors and if one is up, then the other one also tries to bring it to the same stage.

So, if Si is in the up state which means let us say its plus 1, then if Sj is minus 1 in the down state; that means, this energy is minus j, sorry it is plus j. On the other hand, if Sj is in the up state, then this energy becomes minus j, more lower energy configuration.

So, this interaction itself tries to bring the spins in the nearest within in which are in the nearest neighbor, generous neighbor in the same alignment good. So, I want to solve this in the mean field limit, where basically I say that this sum I can replace as Si for Sj. So, I want to evaluate this in the mean field limit.

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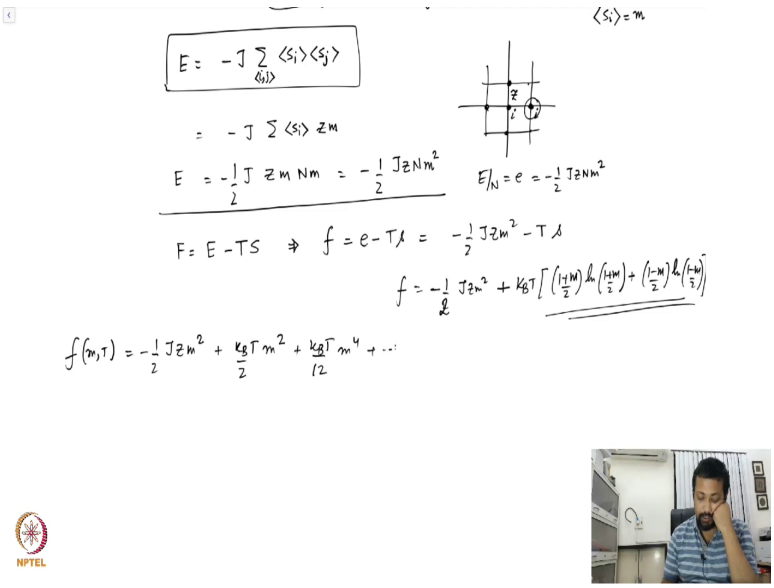

The mean field limit essentially means that I have sum over i and j. So, this interaction I replace by average of Si and average of Sj and already, I have defined that the magnetization per spin which is essentially the average of Si is small m. So, I go to the ith side, so that these two sum over i and j decouples right.

So, I can write down this as minus J sum over Si, I go to the ith side and clearly if I go to the sit in the ith side, it has this lattice point has a certain co-ordination number. Let us say if it is a square lattice, then this is the coordination number we are looking at. So, these are the nearest neighbor points, it has 4 and we will call this coordination number Z.

So, the ith spin is actually if you is surrounded by Z number of spins right. So, therefore, the sum over Z J gives me Z times m and then, I have minus J Z m, the sum over Si now is just N times m. However, now the problem here in this summation is that this you considered as the ith side; but in the next time, you hop in over here and this again you considered as the ith side.

But if the contribution of this side has already been contributed, already been considered over here, so there is a double counting which is involved that is ok with us, except that we bring in a half factor.

So, that this becomes half J Z N m square right. So, this is your energy. The free energy now; so, now, you clearly see that there are two competitions; one is from the entropy, another one is from the internal energy. So, what is going to be the thermodynamic state of this? And that competition between these two is given by the minimization of the Helmholtz free energy which is T minus S and if you write down the free energy per spin this becomes small e minus T times small s.

The small e is minus half J Z m square which we immediately see over here. E over N is equal to small e is minus half J Z N over m square minus T times the small s right. If so, well, one can write down this as half J Z m square we have the expression for the entropy over here, which we are going to use minus sorry this becomes plus K B T 1 plus m by 2 ln 1 plus m by 2 plus 1 minus m by 2 ln 1 minus m by 2. This is the expression of the Helmholtz free energy for particle.

If you are at sufficiently high temperature such that your magnetization is small enough, then I can expand this logarithm over here and I can write down f as a function of temperature as a power series. A little algebra, if you expand this, this is going to give you plus K B T m square K B T over 12 m 4 plus higher order terms right.

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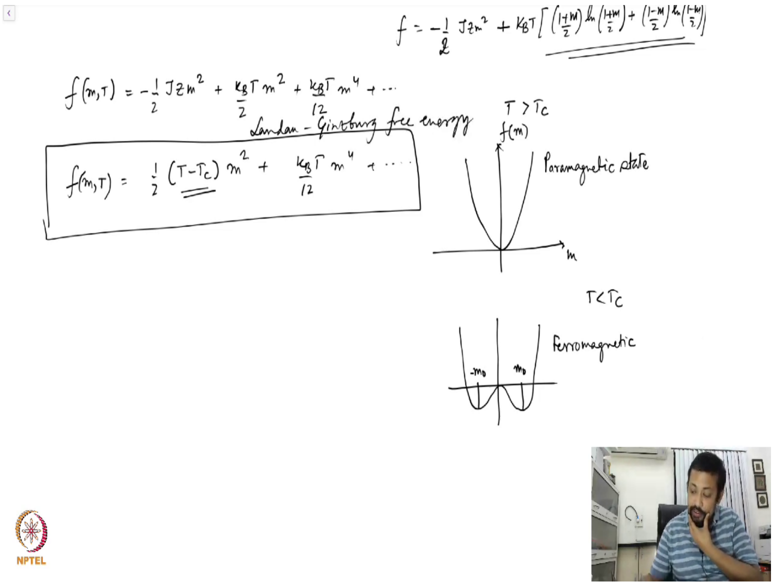

So, this one, I can easily write down as T minus T c times m square plus K B T over 12 m 4 plus higher order terms right. If you now look plot f as a function of temperature, then you clearly see that for temperatures greater than T c this coefficient is positive. So, if I plot T greater than T c, then of course, I am going to see something like this, f as a function of m comma T. If I plot, well let us say let us just write not m comma T; let us write f of m.

If I plot T less than T c, then you see that this coefficient has changed sign and the functional form therefore changes. You develop two minimals at m naught m minus m naught. This is what is called the Paramagnetic state and this is called the Ferromagnetic state. A true ferromagnetism is very very complicated, but it is a very simplistic core strength modeling of ah the ferromagnetic; sorry, the paramagnetic to a ferromagnetic transition.

So, you immediately see that this nice free energy explains your paramagnetic to a ferromagnetic transition right. So, this is your Lambda - Ginsburg free energy. We will not take this further, but just the fact that I wanted to illustrate that starting from this microscopic picture of the spins, we can derive the not only the entropy; but even if we just consider the energy, the interaction energy in the mean field limit, we can actually come up with this very elegant description of a paramagnetic to a ferromagnetic state.