Electronic Theory of Solids

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Lecture – 44
Symmetries of Ising model, Exact Solution

Hello. We are discussing magnetism and in magnetism we have come up to the level of a microscopic model of spins or moments at each lattice site in a lattice.

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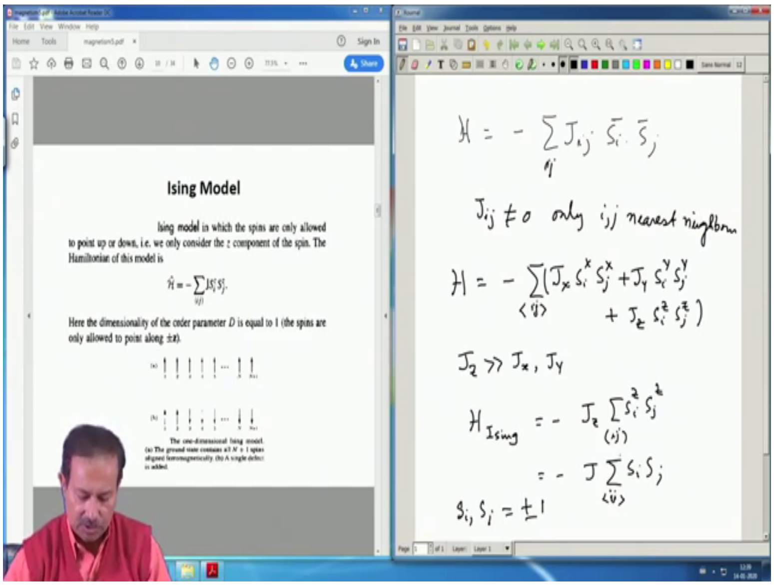

And, this then we found out a description of the long range magnetic order from such models is possible and what we did is that we first wrote the general model H equal to minus J ij S i dot S j and this model then we reduce some where all ij and then we reduce this model to a minimal model which is a simple model which captures much of the physics that we are interested in.

And, the extreme limit of this was that when J ij is nonzero only for ij nearest neighbor. So, that is called nearest neighbor Heisenberg model and that model is it looks so simple, but it is not easy to solve that model and indeed we can solve it only under some conditions in low dimensions and so on which I will come to. So, one extreme case we wrote is that when H could be was written as minus J x S i x S j x plus J y S i y S j y plus J z S i z S j z and then we and let we have made we make it nearest neighbor.

And, then we argued that in the limit of J z much greater than J x and J y this model reduces to the so called Ising model which is minus J z S i z S j z which is customary written as minus J S i S j where S i S j take values S i S j take two values plus or minus 1 each of them all the S i's or S j's take values plus or minus 1. So, and in that case we showed that there are ways to solve this problem. First of all this problem can be solved in mean field theory in any dimension that is something we did.

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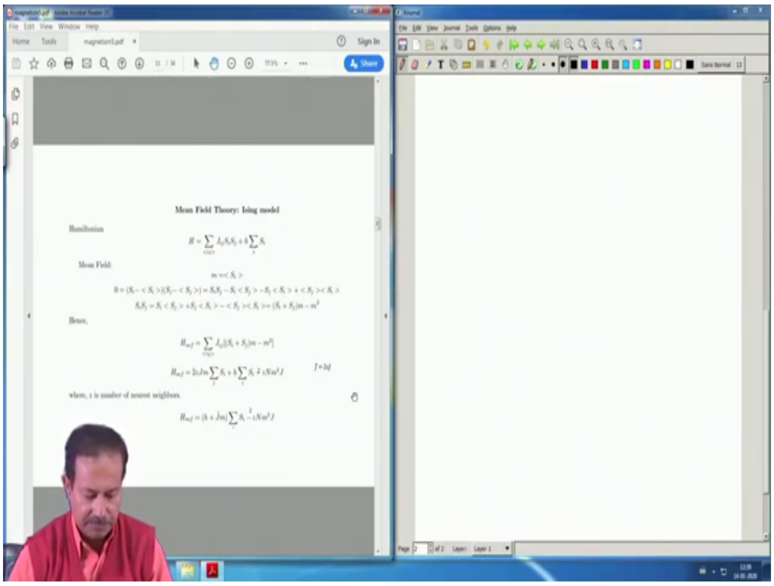

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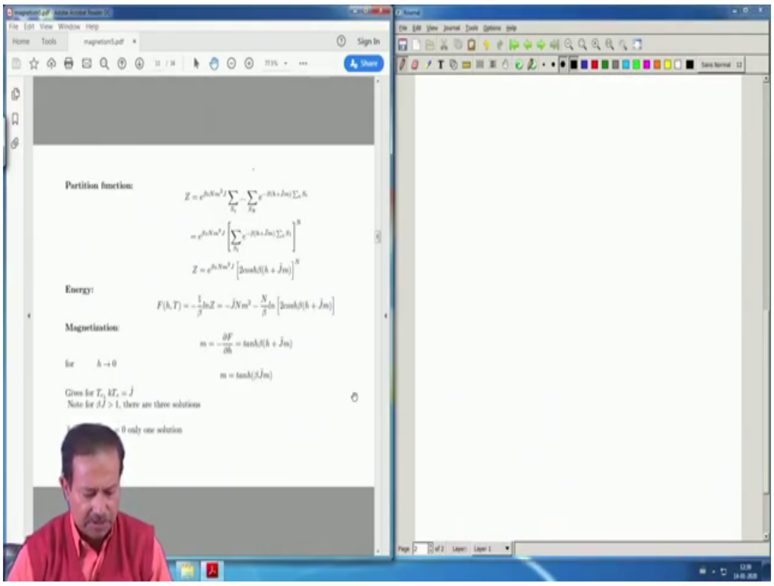

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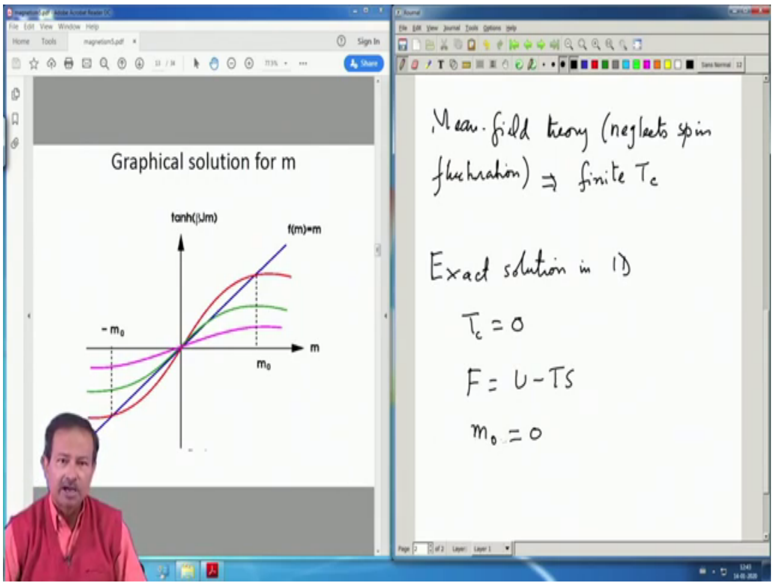

So, that that gave us result which is actually not correct. I mean what is what does it give is that the mean field theory mean field theory which neglects all fluctuations neglects spin fluctuation leads to finite T c below which there is a spontaneous magnetic order. There is a finite magnetic order below T c even at H equal to 0 there is no magnetic field even then there is a magnetically ordered state which is what this mean field theory gave in any dimension.

And, what then we found that the exact solution which can be done in one dimension it can also be done in 2 dimension was done by long back in a (Refer Time: 04:56) calculation and this exact solution in 1D gave us T c equal to 0. So, it said that the it tells us that the in the in such a low dimensional Ising system Ising magnet the entropy is so strong that even at any finite temperature when the entropic contribution starts to play remember your free energy which is what you should consider at any finite temperature is U minus T S, U is the internal energy.

So, at any finite temperature entropy contribution comes into play and that it says that entropy contribution is large and it randomizes the spins and therefore, at any finite temperature you would not see any magnet spontaneous magnetic order this m 0 goes to 0. So, that is a remarkable result in the sense that it tells us that the mean field theory is not a not the right theory. However, as a caveat should remember that mean field theory is still reasonably good theory yet in higher dimensions where the fluctuations are much less.

So, it is not that mean field theory is not used, it is fairly well used and reasonably gives reasonably good results in certain cases particularly when there are large number of nearest neighbors when there are when you are infinite dimension then these kind of theories are quite good and people have been using them for a long time. And, as a first calculation it is easy and it is doable and one does that kind of calculation to get a hang of what is happening. Particularly if you have experimental experimentally you already know what kind of ground states the system has gone into then of course, one can set up a mean field theory to get there.

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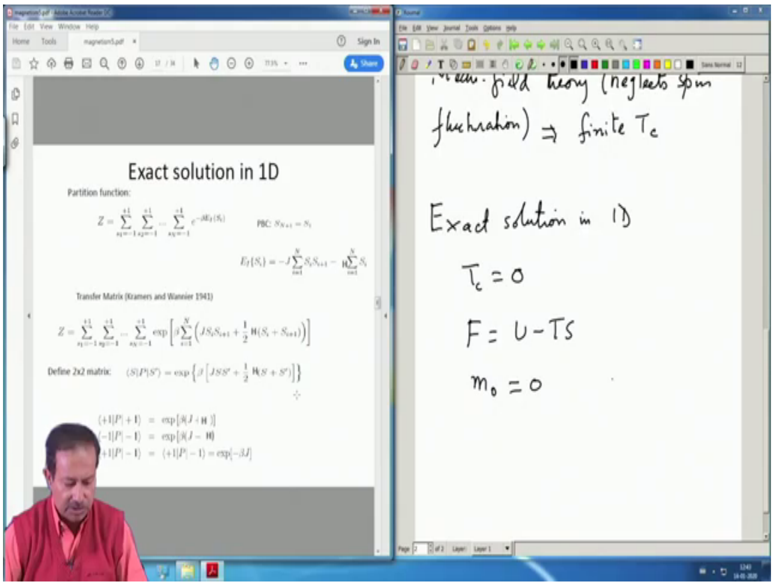

Nevertheless the exact solution let me just show you once more. The exact solution was done using a technique called transfer matrix invented by Kramers and Wannier first wrote down this technique this matrix technique and what I did was that I just reduced the calculation of partition function into a diagonalization of a simple 2 by 2 matrix.

So, that is the enormous simplification that happens if you go by this route. Of course, there are other ways you can do it many books do it in different ways. You can do it you can just look up any book or literature and there are various ways to do it ok. So, this is one way and this also gives you correct result and.

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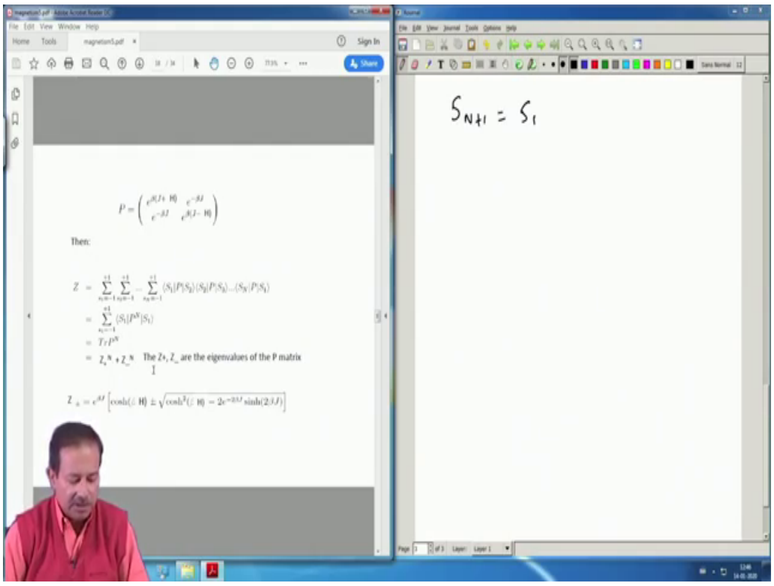

So, what we did was that we just chose a matrix which is whose which is represented by this matrix elements S P S prime and then of course, we calculated the matrix elements, formed the matrix. This is the matrix and then we could write the partition function as a product of these expectation values.

Basically the product of these matrices and the these this matrix product can be simplified further because of the identity that you can sum over these S 2s as every spin internal spin say for the first one and the last one and then you can just go ahead and integrate it out in the sense that these will give you identities complete set of states. So, you are left with only this S 1 P to the power N S 1. This S 1 comes from the periodic boundary condition last S 1 which is which where we assume that S N plus 1 is same as S N S 1. So, the last the last S 1 comes from that.

And, there are we are left with P N number of P matrices in between. So, it is just the S 1 P to the power N S 1 and this is basically the trace of P to the power N matrix. Now, even that we do not have to calculate as I showed, all you have to do is to just find out the eigenvalues and then this just this is the trace ok. So, these eigenvalues are written here.

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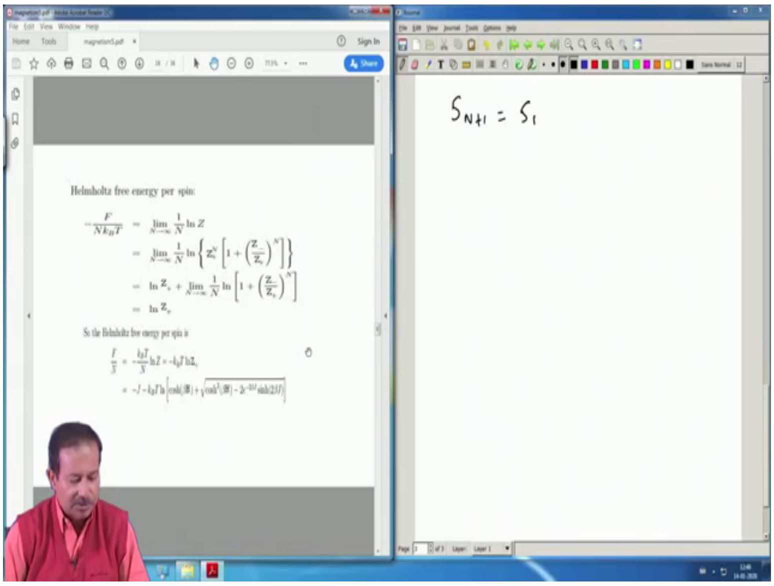

And, now if Z I mean one of the eigenvalues is greater than the other so, you can actually do one more simplification because N is enormously large, so, the thermodynamic number. So, you can only leave with one eigenvalue which is the larger eigenvalue. So, that is how the F by Nk B T is just minus log Z plus Z plus being the larger eigenvalue of P matrix ok.

So, then you can write down the free energy. So, this is an exact solution. There is no approximation in this everything is done exactly and so, you have the exact free energy which is this.

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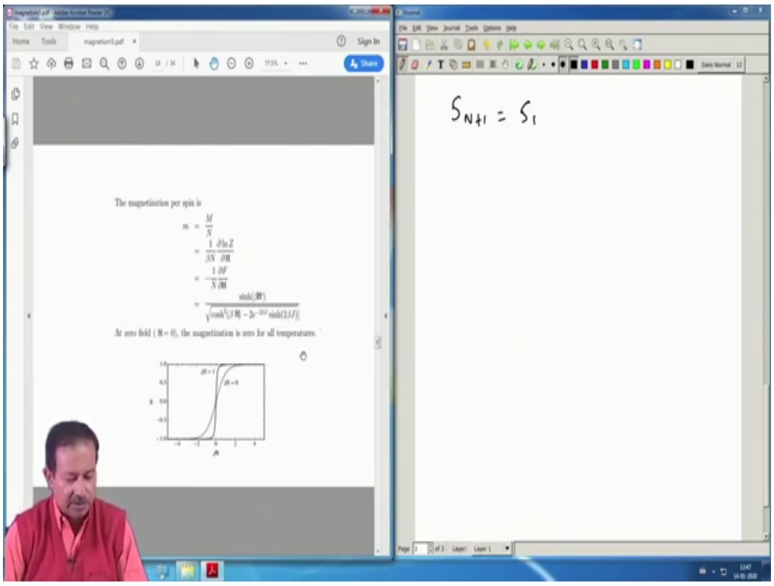

And, that leads to this remarkable result that the magnetization vanishes for any finite temperature as H goes to 0, the magnetic field goes to 0 and that is what is represented here. This midpoint you can see at any finite temperature at H equal to 0 you will pass through this 0. Of course, at finite H you will certainly have other magnetic properties other magnetic values of magnetization in the sense that because H is finite it will induce a magnetic moment in the system.

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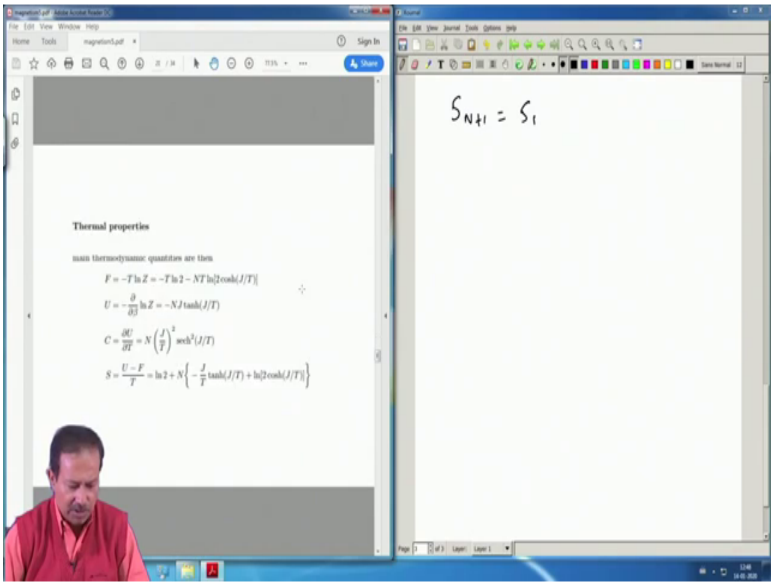

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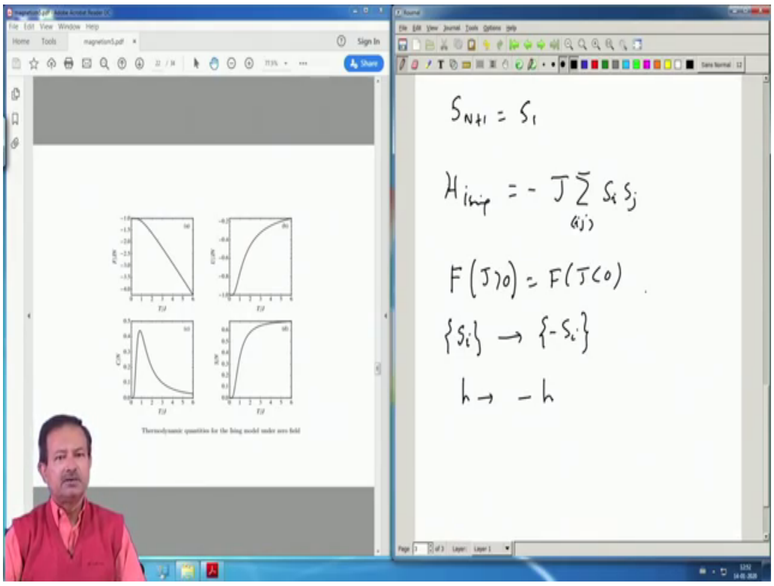

There are certain interesting things that you can actually look up yourself in the Ising model. These are these for example; thermal properties as I said you can calculate thermal properties from this, once you have this free energy of course, you can calculate everything. So, that is what is done here. All these things are calculated you can do it yourself as well, it is just taking derivatives and then you can plot it in a computer and see how they behave. And, specifically in particular is interesting it again has this schottky kind of peak which is which we saw in another two level system earlier.

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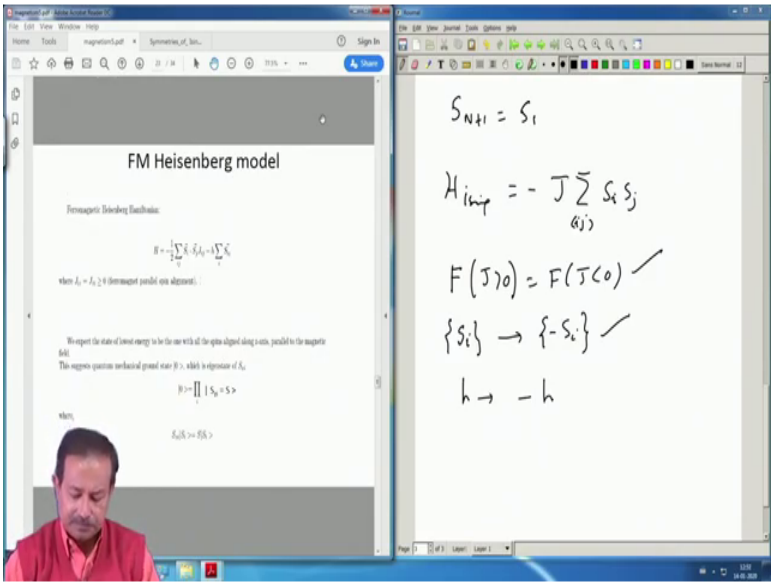

Now, what I will go to is something which is more general and that is the model we started from which is ferromagnetic Heisenberg model. Before that let me just outline a few things about Ising model which are really interesting. One only few things I will outline the rest I will leave you to find out.

The Ising model if you look at the Hamiltonian H Ising say the simplest form nearest neighbor S i S j. In this case S i and S j take values plus or minus 1 plus and minus 1 both. And, in this case you can actually easily show that the you if you if you calculate the free energy for example, or the partition function you will find that your free energy for J positive as is the same as free energy for J negative and that is that means, there is a.

So, there is a symmetry that exists in the this Ising model which is a symmetry that we normally that is why we do not normally mention whether you are in a ferromagnetic Ising model or a non or an anti ferromagnetic Heisenberg model because it is the same thing. The other trivial symmetry is that the S i any the set of a S i's can be transferred to minus S i ok. So, that is another symmetry that is there and so, all spins up and all spins downs is the same thing there degenerate state. So, that symmetry exists in a in this model.

So, this also allows us to make spin H the magnetic field going to H goes to minus H the magnetic field, you can take 2 minus H and then simultaneously if you change all S i to minus S i then your state remains the same you Hamiltonian remains invariant and so, you will you do not need to bother about which direction the spins are you just the idea final result will be the same. The spins will just align in the opposite direction.

So, these are things that one encounters in these symmetries are very important. In any Hamiltonian that you study there are the symmetries that you will encounter and these symmetries tell you a lot because then you know what kind of states you should look for, what are the states you do not need to look for, what are the results you can get from one result by using the symmetries and so on and so forth.

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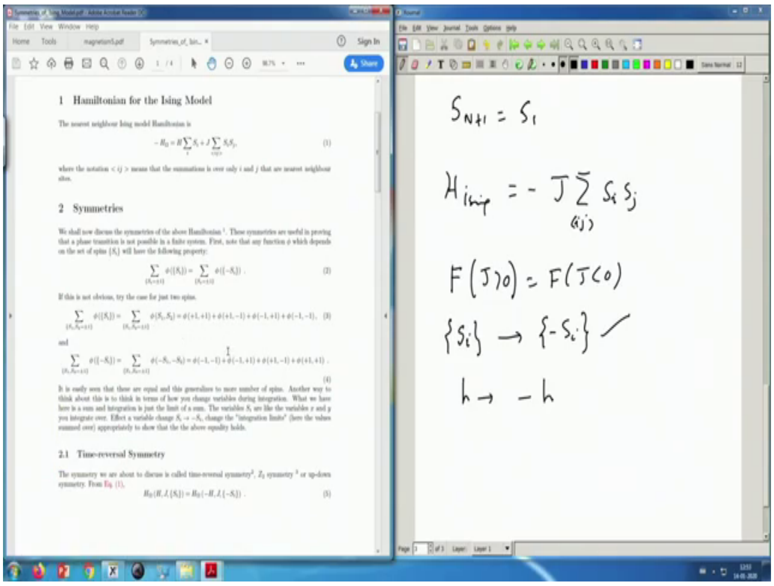

For example, I can show you a lot of symmetries in this for example, you see that this the function f the symmetries are useful this. So, any function which is a function of all these Si's of this mod from coming from this model has this symmetry which I just mentioned. So, this was this is the symmetry and this can be easily shown I mean I did not give you the proof, but it is so obvious that you can actually do it here it is done with two spins, you can do it with n number of spins without any difficulty.

Then of course, this time reversal symmetry which is as I just mentioned that since S i goes to minus S i is a symmetry H goes to minus H is also a symmetry. So, that symmetry means H goes to minus H is a time reversal operation right, the magnetic field goes to negative if you go to the time reverse state. So, that is that symmetry also exists here.

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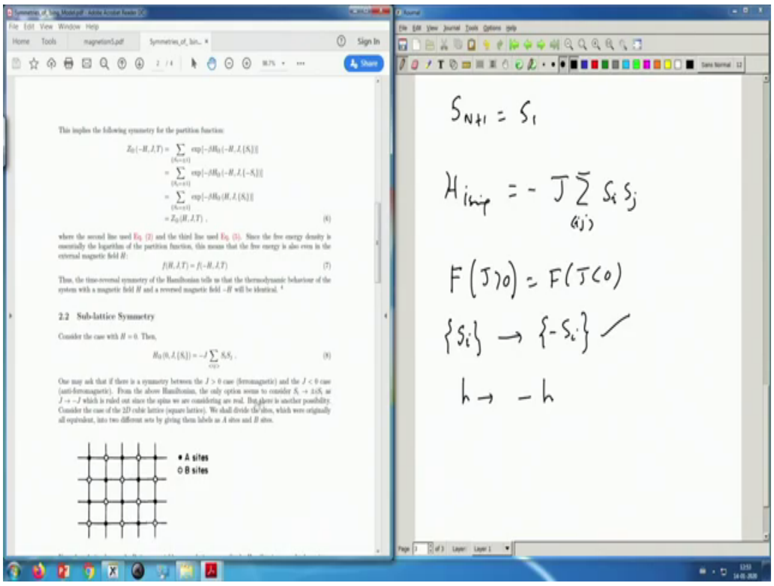

Then there are other symmetries which allow you to as I said J greater than 0 and J less than 0 0 also has a symmetry because then you can just rotate the spins in one of the sub lattice in a bipartite lattice you can do that and you just rotate one of the sub lattice, the spins of one of the sub lattices and then you can show that this symmetry exists.

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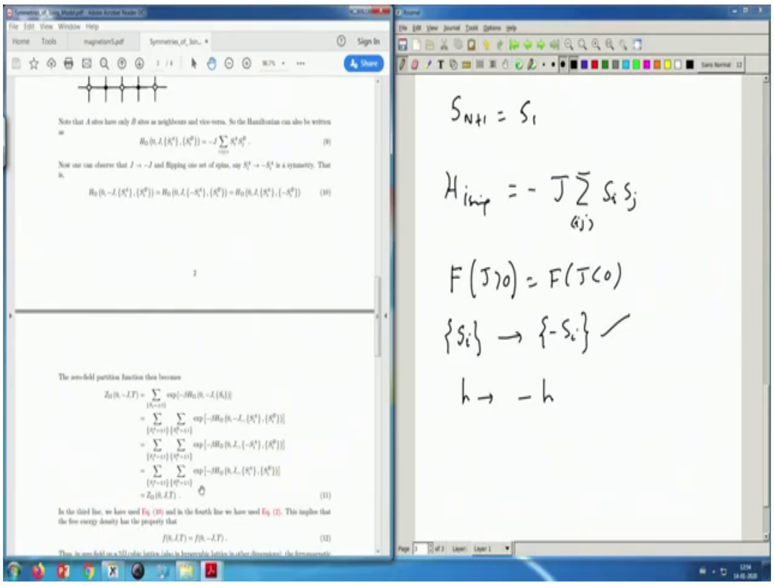

So, the symmetry finally, is that the partition function and for the free energy will be 0 at this is at zero-field of course. If you have a field of course, that field chooses a direction then you do not have a choice, but then you cannot rotate the spins on without rotating the field. So, this is for example, at zero-field minus J, T. So, that is same as zero-field J and T and that is what I have shown here. See, the free energy which is the log of the partition function has this symmetry and that is why it is generally never said that you are dealing with a ferromagnetic Ising model or an anti ferromagnetic Ising model because they are equivalent you can go to one from the other.

So, these are symmetries that are extremely important in real systems, but for more complicated models of course, these symmetries are much more helpful because then you because more complicated models have are more difficult to solve and in higher dimension for example, or in Heisenberg model where all three components are there it is much more difficult to solve the problem and sometimes you cannot solve the problem.

But, if you know the symmetries, particularly for example, most of the times one does numerical calculations on a finite size system and then in that case if you know the symmetries then you can reduce the Hamiltonian to a to a large degree, so that you only have to work with say block diagonal Hamiltonians and that really is enormously helpful in solving this kind of problems; by solving I mean you cannot exactly solve analytically you want to do it on a computer for example. And, once you know the symmetries then of course, your life becomes much simpler. The computational time that is required to solve the problem because much less.

So, and these are useful tools to know the symmetries to be able to use them and that is why I just mentioned some of these symmetries. Keep it in mind when you if you do work on a spin models then try to respect the symmetries and you have to respect the symmetries too and it helps you to reduce your calculation enormously. Let us go back to what we are doing.

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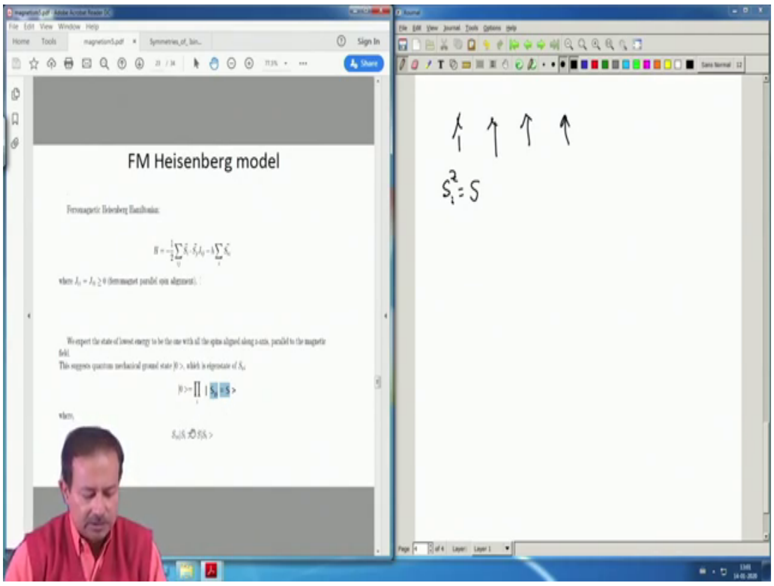

So, I now want to get to a Heisenberg model full Heisenberg model and that is a formidable job actually except that if you have a ferromagnetic Heisenberg model where this for example, in this model if all J ij's are positive, then these spins will try to be aligned in the same direction and the magnetic field of course, chooses that direction. So, we here it is taken in the z direction and therefore, you can you can actually solve this problem quite easily if you have a ferromagnetic Heisenberg model.

On the other hand, if you have an anti ferromagnetic Heisenberg model that is enormously difficult and that is solved only in one dimension by Hans Bethe and that solution is a to the force calculation. It is in 1931 he solved this problem using something nowadays called Bethe ansatz. So, he made some ansatz based on which he could finally, get the exact solution and that is really remarkable. I mean it is a remarkable calculations in the history of mathematical physics and that is still used and that technique is called Bethe ansatz.

Anyway so, that is just one dimension in for an antiferromagnet. So, antiferromagnet remember is a different beast from ferromagnet as far as analytical solutions are concerned even the physics is very different ok. So, the with that digression let me just concentrate on the one that is doable and easy to do and with some physical insight we should be able to calculate the ferromagnetic Heisenberg models ground state. Let us start.

Now, if you look at the this Hamiltonian look I mean if J J's are all positive and then finally, I will take only nearest neighbor J ij again nearest neighbor, but that is not a restriction for ferromagnetic problem, then this I mean that is not a big restriction the big restriction in a ferromagnetic case in the sense that all J ij's are satisfied if you if they are all if they all have the same sign and even if they are long range ok.

So, so what would be the possible ground state? Classically I can immediately see that all spins up is a ground state perfect. So, let us try that for our quantum mechanical case as well ok. So, for quantum mechanics of course, we have to write down the ground state as a wave function. So, that let us call it 0 that is the ground state the suggested ground state, the likely ground state which is analogous to the classical one.

Now, how do I choose all spins up which means that all the S i z values are have the maximum value which is S which is spin half for spin half this will be S equal to half. So, for spin S the maximum value of S z is S and that is the. So, that all up means their saturation there they have their saturation values S z equal to S at every side and so, one takes a direct product of all such states to write down the grammar state. So, that is what is written here in this ket inside the ket I have written S z S sub z i equal to S for all i's and product over all such states.

So, that is the way it is written where we have mentioned also that this if you operate it with S z then you will get the full value S the maximum possible value S that is how this state is defined ok. So, this S i is basically what is written inside this, this I could write as S i, but here I have explicitly written that this is S all S z is are equal to S. So, at every site you have S I, the z component ok. So, that is this state. So, and then operating by S z you will get S ok.

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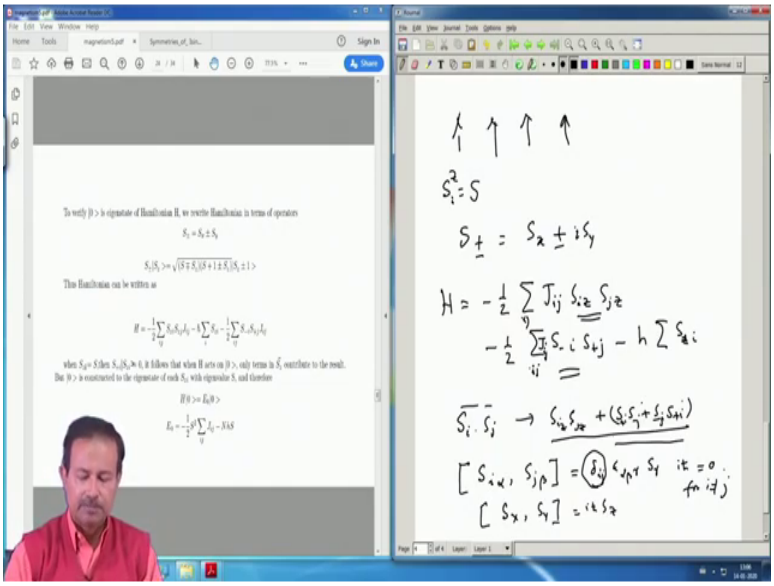

So, we just do as little bit of juggling with the mathematics with the spin algebra. We know that there are these spin S plus minus which is S x plus or minus i S y and i is missing here. So, with that we can rewrite the Hamiltonian in a much better way which is the Hamiltonian can now be written as minus half; see this minus half the half is put again because there is an unrestricted sum i greater than j is not mentioned ok. So, all bonds are counted twice.

So, then we can write this as J ij S iz S jz minus half S i S minus i S plus j into J i somewhere ij I am not using nearest neighbor so far. So, let me just keep it that way. So, this is what I am doing, minus of course, this h S iz S zi ok. Now, what do you how did I get here? You can actually write down this S dot S i dot S j in terms of S plus S iz S i S jz plus this S plus S minus plus S minus S plus, this kind of thing can be done and so, this you can you can try it out yourself it is very straightforward. And, once you do it then this is what I have written here S i dot S j and then.

So, this is basically the transverse component S x S y whatever comes from S x S y is dumped here. Now, if you do it then of course, you will get it get both the terms S plus sorry the plus signs are in the so, ok. So, the plus and minus I am using at the bottom. So, I let me just do that plus minus plus this is how one writes.

So, then of course, and this is i, this is j, this is i, i this is j, this is i and then something that I will do is what I will do is the use of use of these commutation relations right S i alpha S j beta; alpha beta are the components equal to delta ij and then so, this is a Levi Civita symbol alpha beta gamma S gamma times i h cross ok. So, these are. So, this basically tells me this is a complicated way of writing it. All l am I want you to note is that this is just this standard spin algebra that you remember your S x S y equal to ih cross S z. This is the other way of writing it.

The interesting thing is that there is an ij sitting here. So, if you have different sides i and j then this is equal to basically 0 equal to 0 for i not equal to j and that is what I am I am going to use. That is what I will come to.