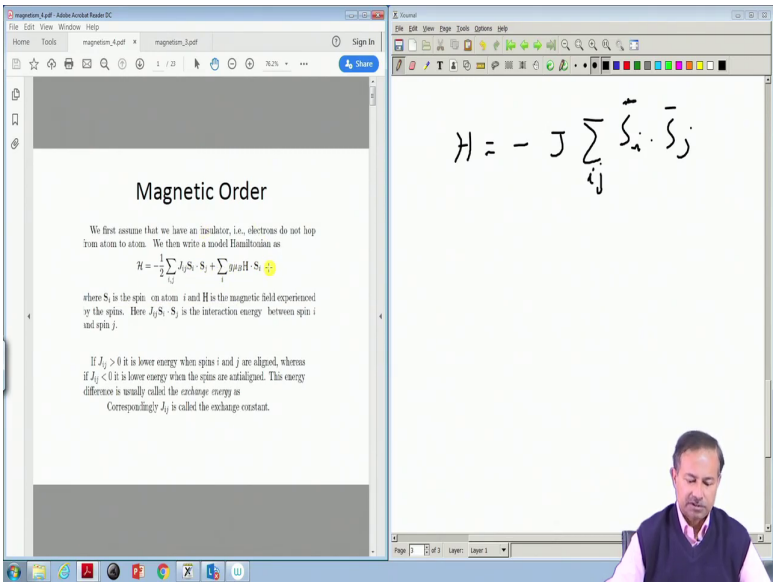
Electronic Theory of Solids
Prof. Arghya Taraphder
Department of Physics
Indian Institute of Technology, Kharagpur

Lecture - 41
Ising Model

So, we have been studying magnetic models exchange interactions and models that led to long range magnetic order.

(Refer Slide Time: 00:35)



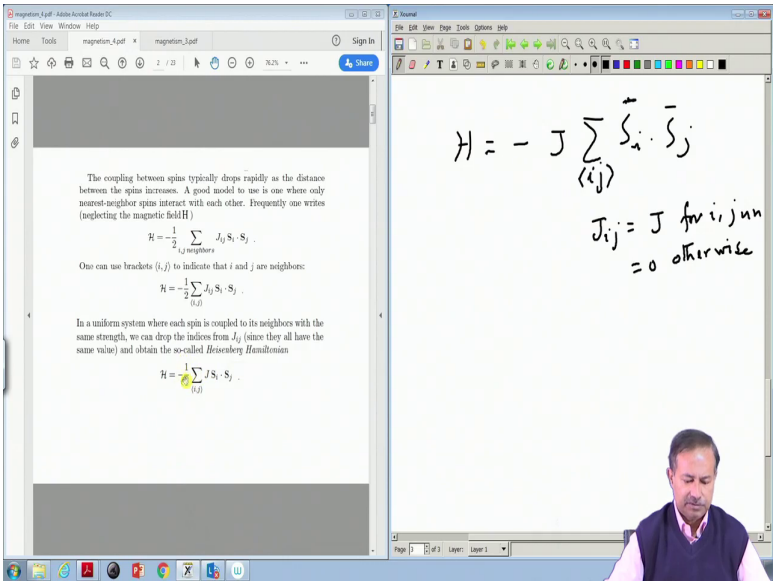
And we found out that there is this celebrated model called Heisenberg model which is typically H equal to minus J S i dot S j. Where, S i and S j are the corresponding quantum mechanical operators for spin S moments and you sum over ij. You can make it i greater than j, so that you just sum only once each point, but nevertheless this is the model. Typically, you can also have a magnetic field in the system, so that magnetic field is the couples to the system and this is g mu B H dot S i this term can presents that.

Generally, one absorbs this g mu B and everything into the into H and writes a model which is just H dot S i. And then sum over always for a constant magnetic field H in a particular direction. So; that means, if the H is in the z direction this will just become H sigma S z sum over all sides. So, as we said before that J ij positive and negative give rise to different kinds

of states; J ij positive will give you a ferromagnet. Whereas, J ij negative will try to misalign the spins align them anti ferromagnetic.

But, if there is a field of course, the field will try to align it in its own direction. So, that will be a competition between the field and the J. If the J is anti ferromagnetic for example, then the there will be a competition. If J is ferromagnetic interaction then of course, if you put the field in the same direction then there is I mean the field chooses the direction. And then the ferromagnet has no competition with the with magnetic field because all spins will align in that direction and satisfy this J.

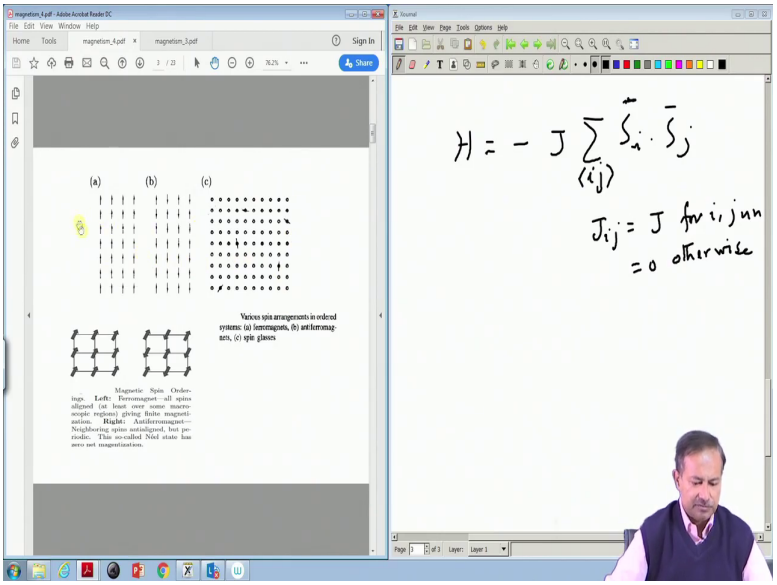
(Refer Slide Time: 02:42)



So, typically as I said before that this i and j are chosen to be nearest neighbor. Because, the interaction drops off as you go to further and further neighbors in your lattice in your solid. And then you can write Heisenberg model with only nearest neighbor interaction. That means, J ij equal to J only for i and j nearest neighbor nearest; neighbor equal to 0 otherwise.

So, that is the way it works and that is the call that is called nearest neighbor Heisenberg model, so this Hamiltonian represents nearest neighbor Heisenberg Hamiltonian. This half you can ignore you can absorb it in J, so those are things that we will do as we go along.

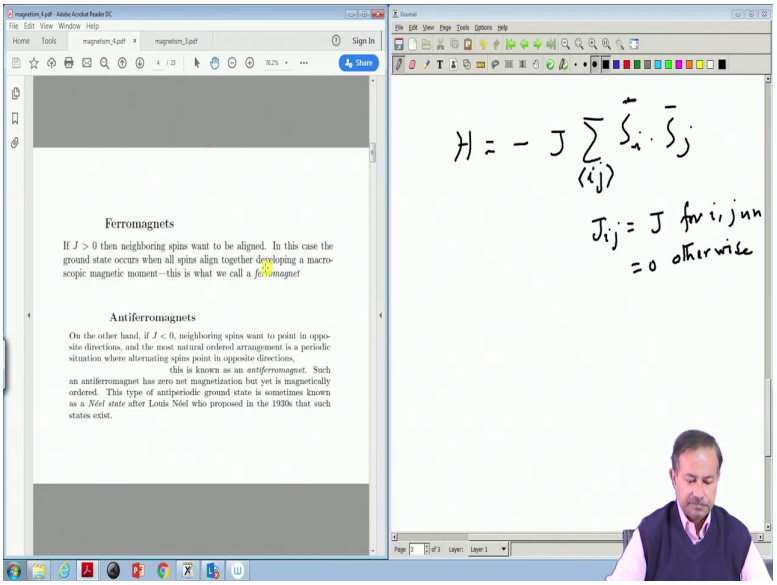
(Refer Slide Time: 03:52)



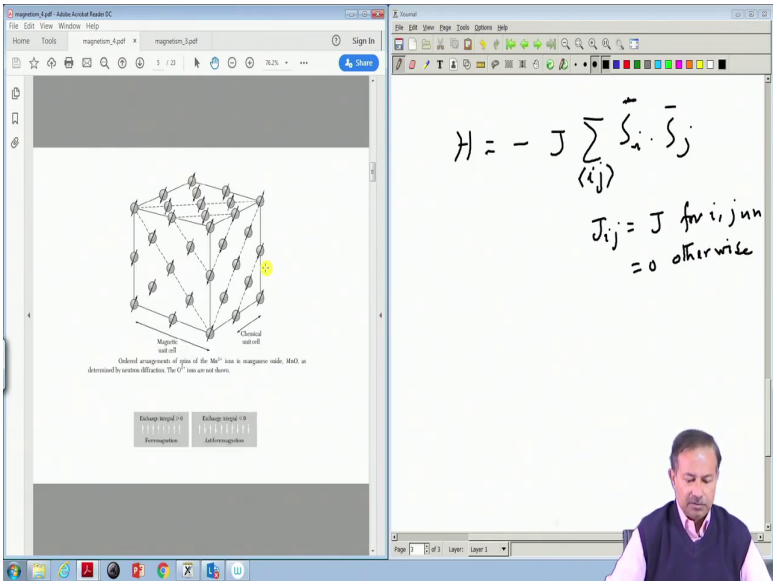
So, these as we have been discussing there are these various kinds of spin orders that come from this interaction. And they provide you a long range order state. The long range order can be of various kinds, this is for example, ferromagnet, this is anti ferromagnet which is which are also shown below.

But, there is a state that is mentioned here as c which is called the spin glass. And I will come back to it is a different kind of state where magnetic moments are in a meta stable state. There is a slow dynamics by which the moments relax the moments are reasonably far apart from each other. And that leads to a state which is dynamic in the sense that the there is no spin freezing over a long time. So, it relaxes to very slowly to its stable state, but that relaxation time could be very large very large ok.

(Refer Slide Time: 05:01)



(Refer Slide Time: 05:02)



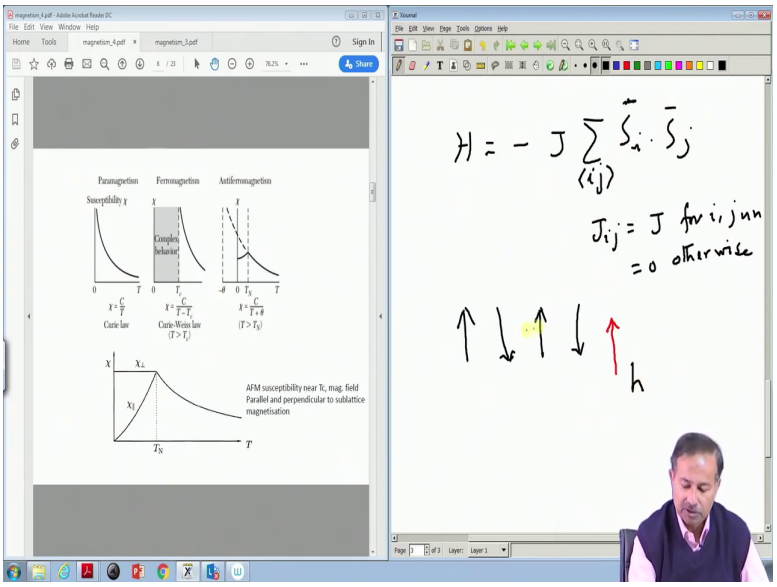
This is an example which is I chose, because you can see that this is an anti ferromagnetic arrangement excuse me, and this is from determine from say a neutron scattering. And you can see that the in the anti ferromagnetic state the unit cell which means the repeating units are doubled. Unit the size of the unit cell is double the size of the chemical unit cell; chemically this atom is manganese, this atom is also manganese.

If you do not look at the spin then you will be your unit cell will be just this will be the distance between the lattice constant that you will use to find out your unit cell. Whereas here for example, the unit cell has to contain more than one atom, two atoms and; that means, the unit cell dimension has doubled.

And this is actually, so even the previous picture you can see in the anti ferromagnet the repeating magnetic structure comes by after jumping two state, two units, two lattice constants not one lattice constant. So, in this case for example, if you had a perfectly paramagnetic state or even a ferromagnetic state you could have chosen your unit cell with just one atom or one moment.

Whereas, here in the magnetic unit cell you have to go two steps to repeat the magnetic structure. That means, your units magnetic unit cell is twice the original chemical unit cell. That has a profound consequences in determining the state of even sometimes metallic or insulating state of a system.

(Refer Slide Time: 07:05)



The way one determines if something is paramagnet or ferromagnet is of course, one is you can do neutron scattering and then actually look at the magnetic structure locally. The other one is that you even from susceptibility see neutron scattering requires you to go to reactor

not for not for everything you go there. If you can determine without going to a reactor is fine.

So, susceptibility for example tells you a lot. So, susceptibility for example, has these different forms for ferromagnetic, for paramagnetic, ferromagnetic, and anti ferromagnetic systems. And this is really interesting that even an MSc laboratory measurement where you can measure this the susceptibility you can actually determine whether something is paramagnetic, ferromagnetic, or anti ferromagnetic.

See the way the Curie law gets modified in a ferromagnet is that there is a C by T minus TC. So, there is this at some instead of going diverging here at T equal to 0 now you have a finite temperature where the divergence occurs. In real systems of course, you would not find the divergence, but there will be a sharply sharp upturn around this TC.

So, the form the way it goes is C by T minus TC an ideal ferromagnets. In anti ferromagnets it goes as C by T plus some theta and at high temperatures and that above the Neel temperature. And that here also this formula is valid for when you are coming from above TC here also you are coming from above TN and this is the behavior that you will see.

So, the other interesting thing about antiferromagnet is that as I said that if you put a field suppose you have an antiferromagnet where spins are aligned this way. And now you put a magnetic field which is say in this direction, let me write small h for magnetic field then there is no confusion with Hamiltonian. So, this h is in the direction of these spins.

And then what will happen is that these spins are now unhappy because they are in their high energy state they are anti parallel to the magnetic field, so they will try to align along the direction. It is also possible that they may not (Refer Time: 10:04) the state may completely change and there are situations where such thing can happen.

And the is just not that these spins align all aligned along the magnetic field that happens for very large magnetic field of course. But there are other possibilities that I will not discuss here, but you can think about it. The other thing is that these sometimes the system itself has a magnetic anisotropy.

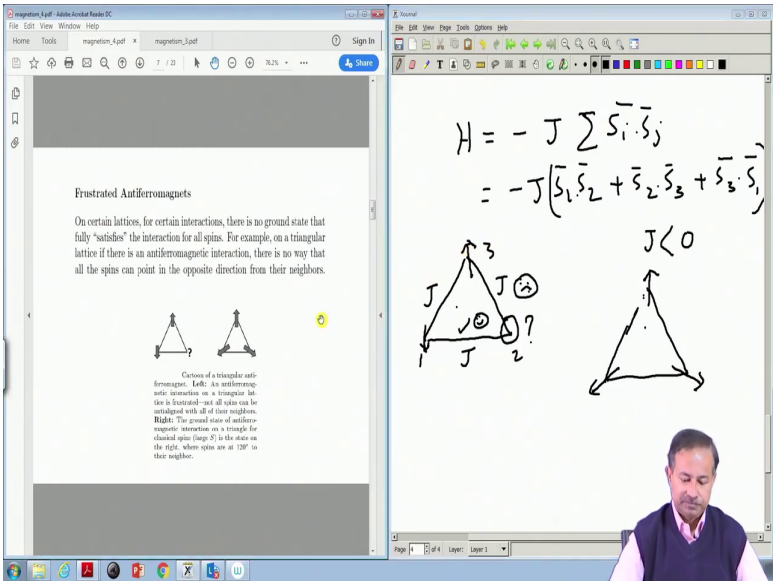
And, so certain directions of magnetization are favored a certain direction is favored and in that case if the magnetic field is parallel to that direction then the susceptibility has this behavior the chi parallel. Whereas, if it is perpendicular to the to the sub lattice magnetization then this is called the sub lattice magnetization. So, sub lattice magnetization has a direction which is up here along this up direction.

So, sub lattice direction magnetization is calculated by taking this up spins and multiplying this down spin moment by minus 1. And; that means, you actually turn it around and make it in this direction and sum over all of them. So, that direction that is the direction the field is here perpendicular to that, the field here is parallel to that.

So, and you can see that susceptibility in the perpendicular direction to the sub lattice magnetization is more or less getting flat whereas, the parallel one is coming down ok. At high temperature of course, its higher temperature above nail temperature of course, this is a paramagnet.

So, you will again get back there is no distinction between parallel and perpendicular. Actually in actual practice it survives a little bit, but I mean those are coming from crystalline anisotropy magnetic crystalline anisotropy and so on. The system itself has certain direction which are favored, but let us not get into that this is the usual picture that you will get in a good anti-ferromagnet.

(Refer Slide Time: 12:29)



So, the parallel and perpendicular susceptibilities will be different below T is TN. So, that is the message that I want you to carry for antiferromagnet. Now, there is this system there are systems which are called frustrated antiferromagnets. Now, frustration of course, is a very common term these days and it is an English term that says that it will not satisfied right.

And it is indeed the case, so they let us take this example and as I remember I mentioned that you have lattices which are bipartite or non bipartite. Now, this lattice for example, is a non bipartite lattice its a triangular lattice. Now, what we have is that in this triangular lattice we are trying to fit in an antiferromagnet.

So, our my Hamiltonian is minus J S i dot S j, S j. So, here it is just minus J S 1, S 2 plus S 2, S 3 plus S 3, S 1 ok. So, this is a equilateral triangle all J's are same and J is greater than 0 and J is less than 0, so that you want antiferromagnet. And then, so fine let us put a spin here and these are spins say for example, these spin have up and down quantum mechanical spins and spin half and say up and down components only. Then the spin this is ones 1, 2 and 3, so this will also be up this will be down because its antiferromagnet.

Now, what will happen to this one? This spin just does not know which way to orient. Because, if it orients up if it is up then this bond is satisfied this will be happy, if it is up then this is ferromagnet. So, this bond will be unhappy whereas, this bond is happy ok. So, that is

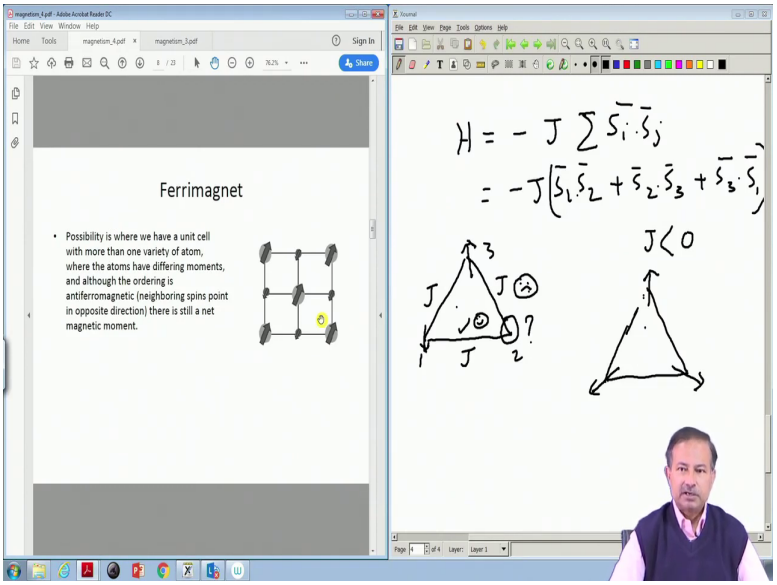
the situation you cannot satisfy this particular spin whichever way you point it will be frustrated because, one of the bonds will become dissatisfied.

So, that is called a frustration. This happens in non bipartite lattices with anti ferromagnetic interactions. In which spins which are the quantum spins here for example, with up and down components. Whereas, if you had a classical spin which can rotate in any direction then of course, you could more or less you could not fully satisfy the interaction. But you could lead to a compromised solution which is the spin is here, this spin is here, this spin is here.

So, they have 120 degree angle between the two between each two. So, this is the best compromised solution you could achieve you could not get 180 degree, but you could get 120 degree. Whereas, here you are lost you just do not know what to do this spin basically is it has both the states which are degenerate. So, it is a doubly degenerate state; if you put up spin this will be dissatisfied, if you put down spin this will be dissatisfied and the energy is the same.

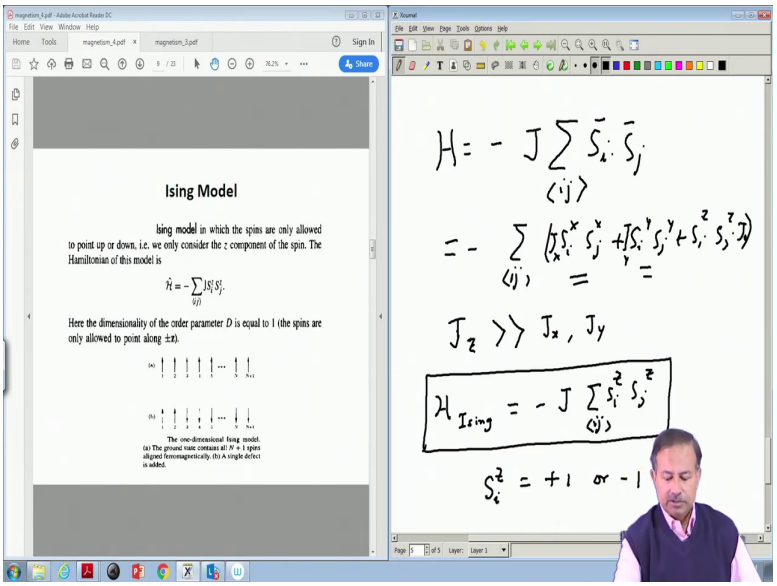
So, this is a doubly degenerate state which is frustrated whereas, this in a classical spin of course, you can rotate the spin in any direction you could get this kind of a compromise solution with 120 degrees angle between the 2. These are called frustrated systems degeneracy is an interesting thing because once you have a degeneracy that is that has higher entropy, so these states carry higher entropy.

(Refer Slide Time: 17:08)



Then of course, I discussed ferrimagnet at some point where you have usually two different atoms in the neighbor. And so, their spins have different magnitude, their moments have different magnitude, and this alignment is kind of alignment is called a ferri magnetic alignment ok.

(Refer Slide Time: 17:28)



So, all now we have discussed a lot of phenomenology without doing any calculations. So, at some point we have to show you how to do calculations with these models and I will just

choose one celebrated model which is the which was written down by somebody called Ising. He wrote this model which is very simple say you can get this model from Heisenberg model in when there is extreme anisotropy for example let me just explain.

So, I have this Heisenberg model minus J, let me just stick to nearest neighbor S i dot S j. So, this means minus J i and j nearest neighbor S i x, S j x these are components x component y component s i y s j y plus S i z s j z ok. So, far so good I have done no approximation.

Now, there are systems where it is possible that these J is not the same in along all directions. And suppose you have a situation where J z. Where one component is one of in one direction j is much higher than in other directions and that direction let us choose z. And so, J z is much much greater than J x and J y this is an of course, an anisotropic situation. The system has this anisotropy for example, say and in that case of course, I can neglect this x direction interactions along the x direction.

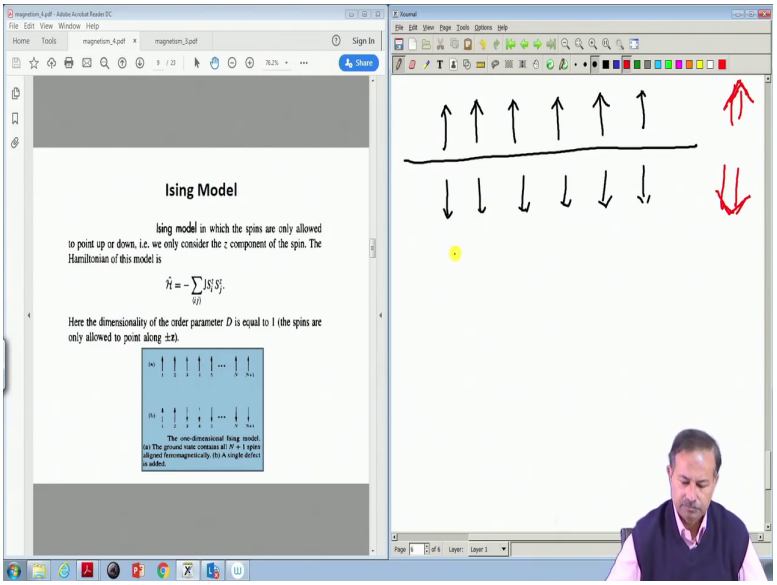
And, so see here what we have written is an isotropic all J, J x J y and J z are same. But suppose they were different I had to write it differently right I had to write it as J x here J y here and J z here. So, and then I am saying that J z is much larger than J x and J y. So, I will write this as the minus J S i z, S j z i and j are nearest neighbor.

So, this model is called the Ising model and it has only one spin component which is the z component. So, when one writes this model one often just does not write this z because its assumed that you have only one component. And S i z takes values plus or minus 1 plus 1 or minus 1. So, that is the model that is for this celebrated model called Ising model.

And we will discuss how to solve these models both approximately and exactly this is in one dimension of course. Approximately you can solve it in any dimension, but for that approximation the one that I will discuss is mean field approximation. But in one dimension one spatial dimension this model can be solved exactly and you can calculate the magnetization the free energy and so on.

And that solution is really interesting because it tells you a lot of physics about such models. Before I go to the discussion of that solution let me just outline the one dimensional Ising model pictorially which is done here this one for example.

(Refer Slide Time: 22:11)



So, you can have a situation like this all spins are up this is in one spatial dimension because your spins are aligned along one direction. If I had a two dimensional two dimensional model I can I have to put spins here also.

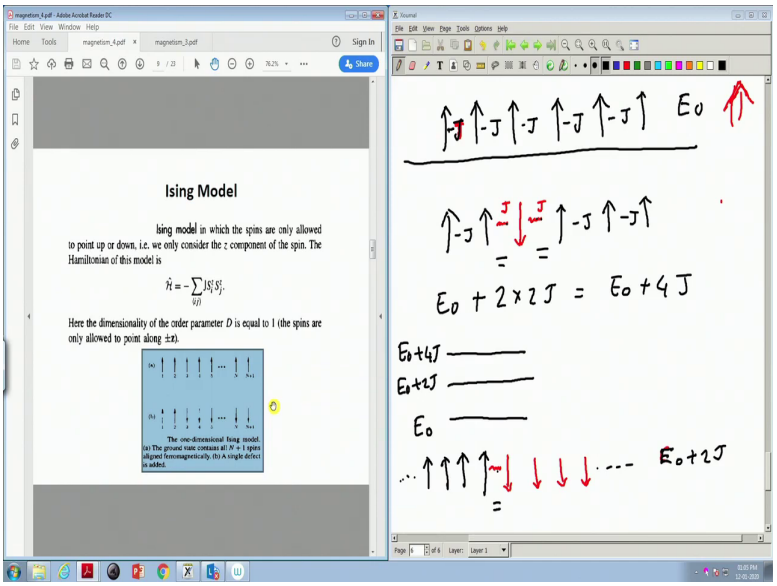
One thing you should realize that the spin space and the real space where the spins are very different things. See in spin space the spins are quantum mechanical objects and they have S x, S y, S z component in the spin space. So, and for quantum mechanics for spin half for example, they follow S u two algebra. If this is real space I can have a situation where spins have S x S y S z all components, but the real space is one dimension that will be Heisenberg model in one dimension.

So, you should be very careful when you it is just a matter of practice you should just remember when we say one dimensional model. That means, the space dimension is one dimensional the space in which the spins are living they are embedded is the moments are embedded, the atoms are the atoms that carry these moments is one dimensional.

So, let us just consider this one dimensional model where the spins can only have two directions or say down spins can be down. As you can see these two states have the same energy cannot distinguish between them in terms of the Hamiltonian they are degenerated states.

Nevertheless let me just, so this is one state which is all up, and this is one state which is all down both are ferromagnet and both are both have the same energy. So, let us stick to just one dimension. So, in this case for example, in one dimensional situation this is my lattice, and this is the spin configuration, and this is the ground state.

(Refer Slide Time: 25:00)



So, every bond now has this energy J plus J. So, if the every bond has this minus J energy because the spins are parallel and they are plus 1 the spins are all plus 1. So, all bonds have the energy minus J from the Hamiltonian you can easily see that. One question which is interesting is that what is the next excited state?.

Which state? For example, lies just above just the next one above this state see this is infinitely extended on both sides ok. So, this is an infinite lattice there is no boundaries or you can just put a periodic boundary condition and make it infinity again it is clear. So, nevertheless whatever the situation we are dealing with in Ising model with only is one spins can only take plus 1 and minus 1 values and it is a infinite system.

The question is this is the ground state of course, for we know its clear from here, but at 0 temperature of course, you will land up in this state this is at least the lowest energy state there is no doubt. Now, I want to create the first excited state of the out of this and this is

something that most often you will one what one does is that one just takes a spin and just turns it around and makes this state.

This is obviously, a one choice of an excited state because now these bonds are this side these bonds are unhappy these two bonds have their Js are unhappy. This Hamiltonian is unhappy the energy here is now plus J all the others are minus J. So, if this state has energy E 0 this is an infinite number of spins is infinity.

So, this state will actually have two spins being dissatisfied it will rise this energy by 2 J this was minus J and became plus J. So, 2 into 2 J so for E 0 plus 4 J, so from minus J you brought it to plus J. So, each of these broken bonds these are called broken bonds or unsatisfied bonds will cost you two J amount of energy and two of them are broken, so you will get this.

But is this the first excited state is there any, so you are saying that this is I am saying that this is E 0 and the next one is E 0 plus 4 J. So, this is correct it is not true actually, let us see what can be another state. So, let me again plot write down the spins, now I of course, turn this spin down. But I keep all the other spins on the right down as well and all the others all the spins on the left up as well this is again infinite lattice. So, now, you see how many bonds are broken? There is only one bond that is broken now this one.

So, this is an energy which is E 0 plus 2 J. So; that means, there is a state in between whose energy is E 0 plus 2 J. So, that is; that means, that this is what is shown here in this b picture on the left hand side. That instead of creating two defects you have created two defects in the top figure.

Whereas, in the bottom figure see in this my the way I have drawn in this figure you have created two defects; one here, one here instead I have created in the bottom figure there is only one defect. So, this state is represented in b in the left hand picture. And this is the first defect state that you can this is one; this is one defect state and this is the first excited state you can have over the ground state.

So, that is what we will do in the next class we will discuss how to solve the problem of to find out the ground state. And of course, also since we will solve the problem we will find out

the finite temperature situation whether that ground state survives in finite temperature or not. Because, there are thermal fluctuations at finite temperature, and from an exact calculation one can do that from a mean field theory calculation one can approximately do that in any dimension.

For an exact calculation we have to stick to one dimension. I will also discuss little bit of the symmetry of this model from the symmetry you can actually guess a lot of things. And little bit of that I will do and then carry on doing the solution and then finish Ising model.