Electronic Theory of Solids
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Lecture – 42
Mean Field Theory

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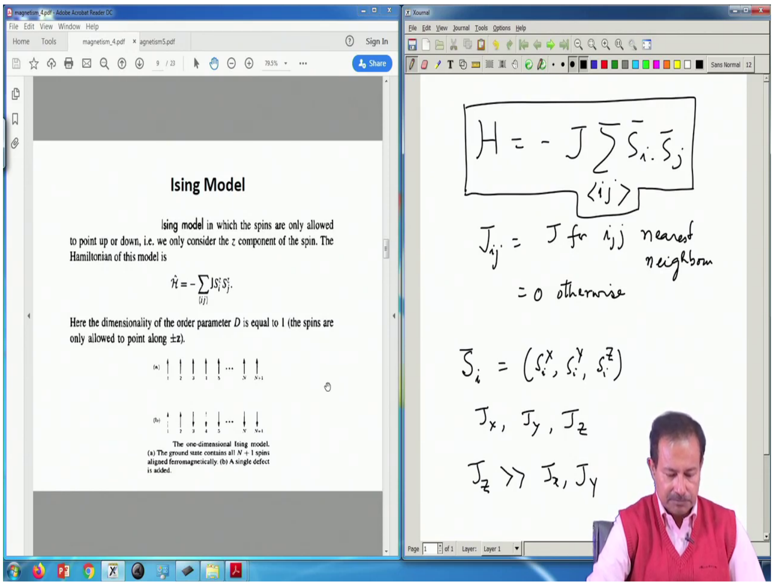

Hello and welcome. We have been discussing various spin models and we started from this celebrated model which is the Heisenberg spin model, minus J S i dot S j, where this symbol at the bottom sum over ij means that you are summing only over nearest neighbour because J ij equal to j, for i and j nearest neighbor and equal to 0 otherwise.

So, as if the J ijs are defined on a bond. So, from this what we mentioned was that this kind of a model requires two things, two information to start with, one is the lattice on which the spins or the moments are residing that gives you the underlying lattice, the geometry of the lattice. For example, you can have a one-dimensional lattice, you can have a two-dimensional lattice. In two-dimension you can have various kinds of lattice square, then triangular, hexagon and so on, honeycomb.

So, then on that lattice the spins are sitting, they are residing, and spins are not moving they are just localized at every side. The other thing that I mentioned as the spins can have all 3 components, S i x, S i y, S i z. Even in an one-dimensional lattice spins can have all components. So, you can define Heisenberg model on a one-dimensional lattice. Spin, the components of spin has nothing to do with the dimension of the space in which the dimension of the real lattice in which the spins are embedded. So, these two things have to be separate. So, two informations are required, one is the how many components of spin are relevant and what are the corresponding J x, J y and J z and the other thing that you need to know is the on what lattice are these spins residing. So, these two informations are supplied. And once that is supplied then one can write down the corresponding model and solve and go on working with that model. So, that is the whole program of solving or working with spin models.

There is a caveat here that this J ij equal to j which is only surviving for nearest neighbor bonds is not necessary, one there are models one can use them to where the J ij are longer range, at least second neighbour, third neighbour interactions are not uncommon. But we are at the moment we are studying with the nearest neighbour J ij.

In that I mention that there is a extreme limit of this model in case of extreme an isotropy where J z is much much greater than J x and J y. And that model is called the Ising model. So, in that model as we shown on the left you only have this z component of the spins surviving. The space dimension can be anything 1D, 2D, 3D, what kind whatever the lattice you are interested in you can put it put this model on that lattice, ok.

So, then I sort of started working on Ising model and I mentioned that there are these interesting of things that you can do with Ising model and in the one-dimensional case where the space dimension in which the Ising model is defined it is just one you can have two states which are degenerate which is all up on both sides going to infinity and all down.

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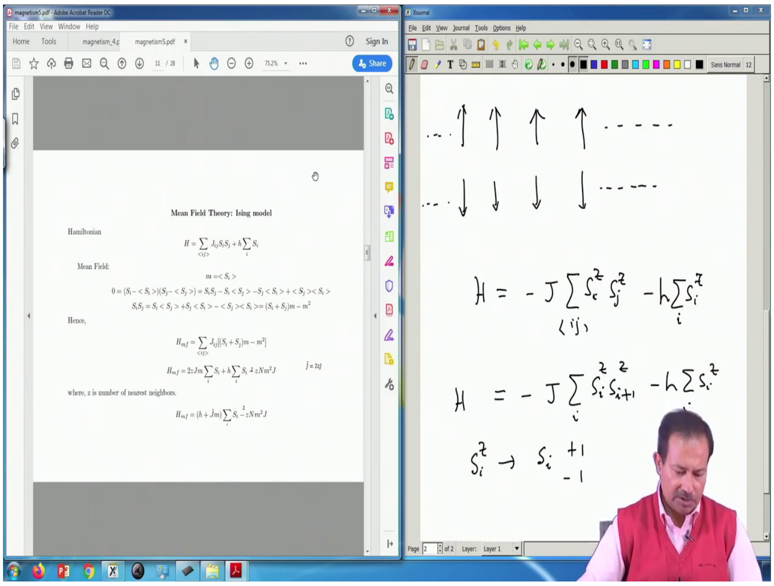

So, you can go to either of the two states for example, when the result is a Ferromagnet. You can also add a field to this, so that the Ising model for example, minus J S i z, S j z minus H times sigma or you can take a plus J if you want hardly matters. So, this can be H times S i z, ok. So, that the spins will try to align along the z direction.

So, the all these mu b g those factors are taken inside the absorbed inside the magnetic field. So, that you do not have to bother with those numbers. At the end of the day when you need the numbers we can put them in, ok. So, this is for example, is Ising model with a magnetic field and one can then have a Ising model in one-dimension, so 1D Ising model is basically defined as minus J S i, S i plus 1 minus H S i z because in that case you only have one direction to consider and this is a standard way of writing.

This sum if you do not; if you do not restrict it to i greater than j or do not repeat a particular bond twice then this is the x, this is correct. If you allow that then you have to put 2 here. But these are things that can always be absorbed inside J, your magnitude of your value of J can be suitably adjusted. So, do not bother about such factors. Just think of this as a Ising model.

This S i z being only one component, it is often just written as S i, we have with a power value plus 1 or minus 1, ok. So, that is how the Ising model is mostly written. In some books you will find it is written with sigma. So, same always the same thing they take the values 1 plus 1 and minus 1.

Now, the way one can solve such models is the as I said there are many many different types, and different types of approximations one can make. And one which is on the most common approximation that is hugely popular is the mean field approximation. So, what does the mean field approximation do? Well, in terms of physics it basically neglects fluctuations. In Ising model for example, the one that is for example, written here one can make that assumption as I will just show that the fluctuations are 0. What are the fluctuations in an Ising model? In an Ising model the fluctuations are thermal fluctuations.

So, the thermals at any finite temperature there will be thermal fluctuations, so that fluctuation is being neglected. Then what does it mean? It means the suppose so this model for example, this model is a translational asymmetric model because no bond or no spin is different from the other spin, right. This is the way I have written it.

If j i is equal to j for nearest neighbors every j is the same for any bond, every S i is you can take any spin and that is no different from any other spin. So that means, there is an average you can define which is independent of the site. So, this is your m is an average, and if you sum over all such sites you will get N times m and that is also the magnate total magnetization of the system.

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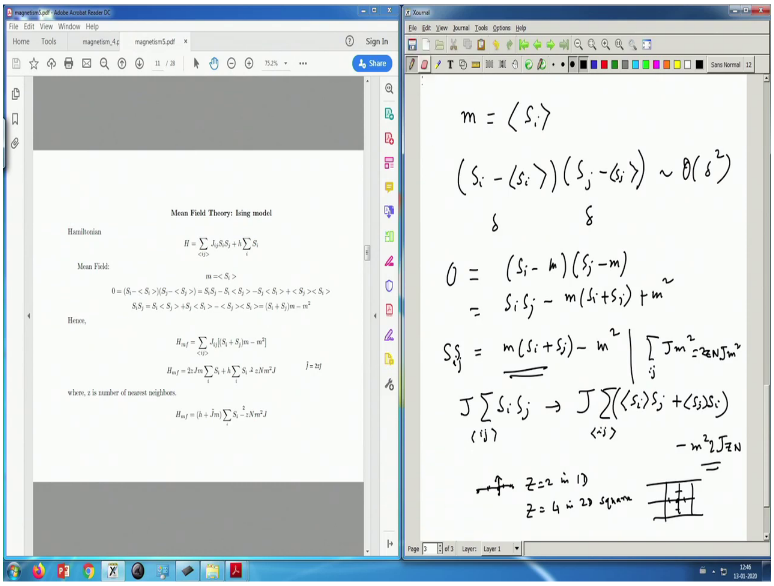

So, if you do their approximation then neglecting fluctuation means you just subtract from every S i, it is mean value and so this is the deviation from the mean, so delta. This is another deviation from mean, so this thing is of the order of delta square.

And presumably it is a very small quantity unless your temperature is very large. And in different models this has different values, but ideally if you are at low temperatures these are values these fluctuations are small and you can neglect terms of order delta square. So, if the if you do that then this 0 equal to on the left you have you have done it, it will become a S i minus m, sorry this is S i and S j which is basically S i minus m into S j minus m equal to S i S j minus m into S i plus S j plus m square, ok.

So, S i S j in this approximation, S i S j equal to m into S i plus S j. So, I bring it to the other side minus m square, ok. So, that is the; that is the approximation that one does. So, one will replace these terms like J S i S j by terms by terms like S i S j plus S j average S i which is done here, because this average is basically m minus.

Of course, this m square term times the number of sites times z times n, I will come to this. And if you have unrestricted then you can put a 2 here, ok. So, that is the approximation one is talking about. So, what happened is that, so for example, at each side the spin interacts with its 4 nearest; so, in one-dimension for example, let us just stick to one-dimension, in one-dimension. Remember this mean field theory does not really care about the dimension, but you let me just show you in one-dimension, but then I will leave the dimension as free.

So, for example, in one-dimension this spin here has this S i S j interaction is replaced by this spin times the average value of this spin and all these, this one and this one. So, S i S j is this one into average of these two, and the number of such terms is in this ij sum if it is unrestricted is the basically it counts the number of bonds. So, it is the z is the number of bonds on twos only nearest neighbors. So, that is 2 here.

So, z equal to 2 in 1D. In 2D square lattice z equal to 4 in 2D square or cubic layer is generally called hyper cubic lattice. So, square or parallelogram whatever. If it has this kind of a geometry then you will have every side has 4 nearest neighbor bonds.

Now, if you have double counting as it is done there then you will have to put a 2 here. So, that is this number. So, these this came from just m square, J m square sum over i j. So, that will give me 2 J, 2 z N J m square, that is the term I have written here, ok. So, this is how the approximation mean field approximation goes.

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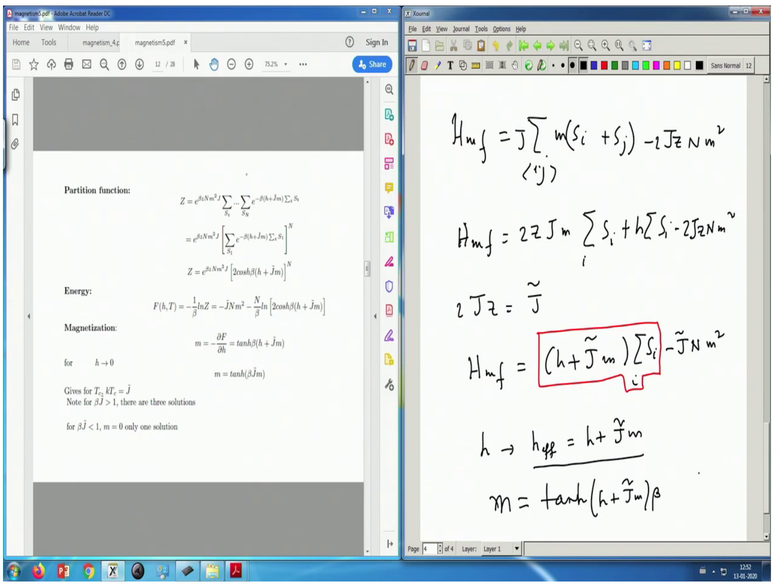

So, what one gets is H mean field therefore, is sum over ij, let me just take out J, nearest neighbor J, J m S i plus S j minus J 2 j z N m square N is the total number of sides. So, that is the term that is written here on the left for example. Here this H mean field is this.

Now, you this I as I said there is nothing to distinguish i with j except that i and j were nearest neighbors. So, we can just to replace this by H equal to 2 z J m sum over i S i because this sum i, one of the indices is free now i or j, for this one j is free, for this one i is free. So, it basically counts the number of sides and it is also the number of nearest neighbors.

So, this plus h times S i minus 2 J z N m square. Now, write J z equal to just define it. So, that you absorb all these constants into a redefined J tilde that means, H m f equal to h plus J m into S i minus J tilde N m square. Now, if you look at this term this one, this part of the Hamiltonian, this is saying that you all you have done is you have replaced your magnetic field by an effective magnetic field which is h plus J tilde m, proportional to the magnetization.

So, that means, what has been done is that the effect of all the neighboring spins on a particular spin say S i is replaced by as if this other spins are giving a magnetic field it is just adding to the external magnetic field h. So, this is why it is called a mean field. It is mean because all the spins are all the neighboring spins are giving same field m times J tilde. So, that is why it is called the mean field.

So, these effect of all the other spins, the interaction term which is J S i dot S j the actual Hamiltonian is replaced by a by taking one spin and replacing all its J spins nearest neighbor spins by their effective field on that spin. So, as if you have a new magnetic field which is a external field plus J tilde times m, the field coming from the other spins. So, that is why it is called the mean field. And this field is same everywhere because it has no site index as you can see, ok.

So, this now is a Hamiltonian which we know how to solve because S i takes only two values plus 1 and minus 1, and we are actually calculated the partition function for such a system in a magnetic field when we did the Curie problem, Curie susceptibility. So, that same partition function will work here, the same equations will also be obtained here with a different field. The field being dependent on m itself, that is the difference.

So, one just goes about doing the same thing. You say again get that cos hyperbolic factor, then you if you want to calculate magnetization then you will just take a derivative of F the free energy with respect to h with a minus sign and the result is this m equal to tan hyperbolic beta h plus J tilde m into beta. In the previous case, in Curie's law we only had h times beta which is the external magnetic field h. Here the magnetic field is replaced by a quantity which is J tilde m which itself depends on m.

So, this is a transcendental equation on the right and this is just m on the left. So, m depends on itself. So, this is such situations are called self, these are self-consistency equation because you have to self consistently determined the correct value of m. So, that is the whole game that one does here. So, if you only have had a field without this J tilde m you would just have tan hyperbolic h times beta.

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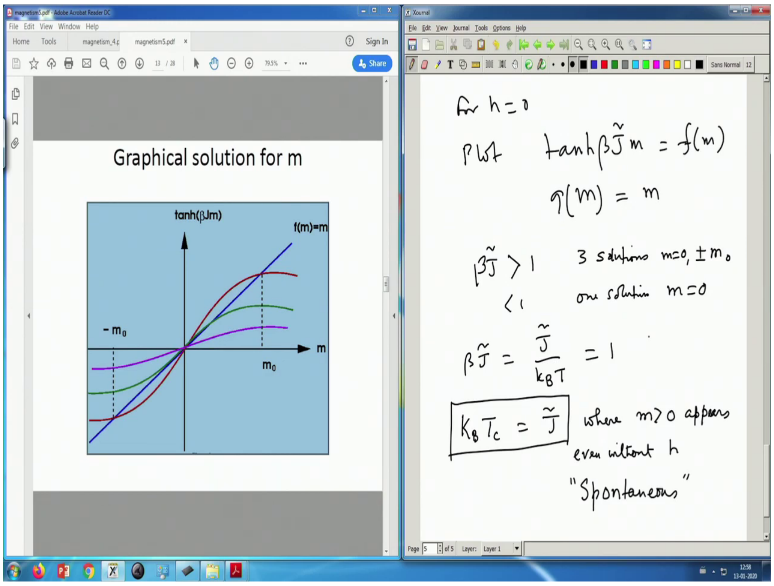

So, let us now try to find out how to solve it. I mean the there are many ways to solve it. The one which is very popular in many many places you will see and it is a very physically quite transparent. These you just look at the solution for from a graph. How do you plot it? So, this is a for example, h equal to 0 you are going to plot it, this is being plotted at h equal to 0.

So, at h equal to 0 your equation is basically m equal to tan hyperbolic beta J tilde m and that equation. So, two equations you plot, one is tan hyperbolic beta J m versus m, right hand side. So, for h equal to 0 plot tan hyperbolic beta J tilde m. So, this is your f, some function of f m, some function of m. And also plot another function which is m which is sum g of m equal to m. See which is basically a straight line with slope one, and the intersect of this will be the solution. So, that is as simple as that.

Now, how I mean how does one find out the solution? It is very straight forward. You can see that these different graphs of different colors on the left in this then you can see that the there are this act around m equal to 0, there are tan hyperbolic beta J tilde m has a slope which is proportional to beta J tilde, close to J equal to 0, close to m equal to 0. Now, that means, if beta J tilde, the slope is more than 1 then you have 3 solutions. If it is less than 1, you have only one solution which is m equal to 0 and that is exactly what is shown here. 3 solutions are m equal to 0, plus minus m naught.

So, the depending on the value of beta J tilde if it is more than 1 you have 3 solutions, if it is less than 1 which is for example, the purple curve and the red curve has beta J more than 1 beta J tilde, purple curve has beta J less than 1 and the green curve is just above to when beta J equal to 1. So, as you can see this as beta J approaches 1, these solutions m naught and minus m naught the symmetric and they start approaching towards m equal to 0.

So, beta J naught, beta J tilde is equal to J tilde by K B T. So, that equal to 1 is the point where you go from one solution to 3 solutions. So, nonzero m solutions, remember this is magnetic field equal to 0, external externally there is no magnetic field, so h small h was 0. So, even with that depending on this value J tilde by K B T that means, J tilde equal to K B T, K B T equal to J tilde, there is a possibility, there is a situation that you have a finite magnetization solution either plus m naught or minus m naught..

Remember, up and all up and all down are equivalent. So, plus m naught and minus m naught are basically degenerate, we can only consider the one solution, so plus m naught say. So, that is a finite m naught solution. So, this is write written as K B T C equal to J tilde, where m m not equal to 0, m greater than 0 sorry appears even without m greater than 0 appears even without h, external magnetic field. So that means, this is called spontaneous magnetization.

This was not the case with paramagnets remember. Paramagnets you require an h to produce a magnet to magnetization. Here you can have depending on what temperature you are there is a play temperature which is given by T C at which you have a nonzero m solution which is stable and which has a lower energy.

And this is the so called critical point at which you have a; so, you have a finite temperature point where you have generate a spontaneous magnetization and as you increase the temperature from below the magnetization slowly decreases at T C it becomes 0 and then it becomes. So, it continuously goes to 0 at T C and then it remains T C for any temperature greater than T C.

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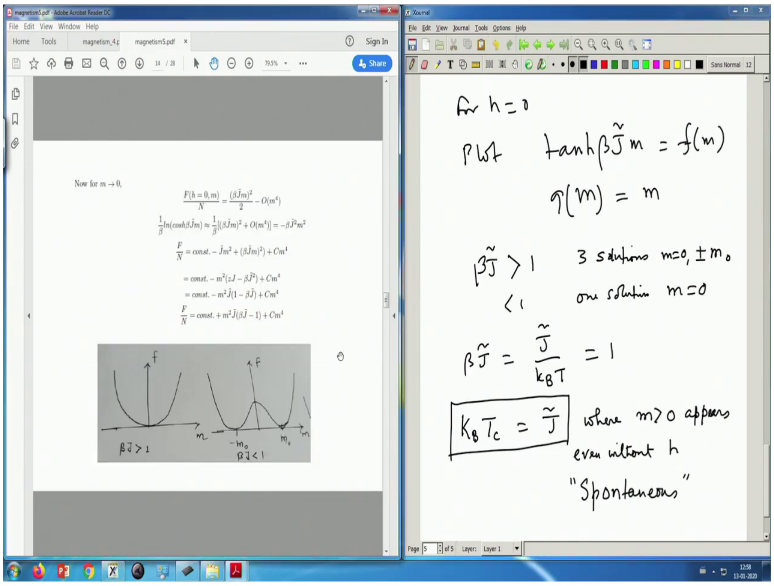

So, that is the mean field solution that tells us. One can do more than that which is what I will do in the next view graph, and we will come to it in our following, in the following discussion.