Introduction to Statistical Mechanics

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Lecture - 17
Correlations and Mean Field

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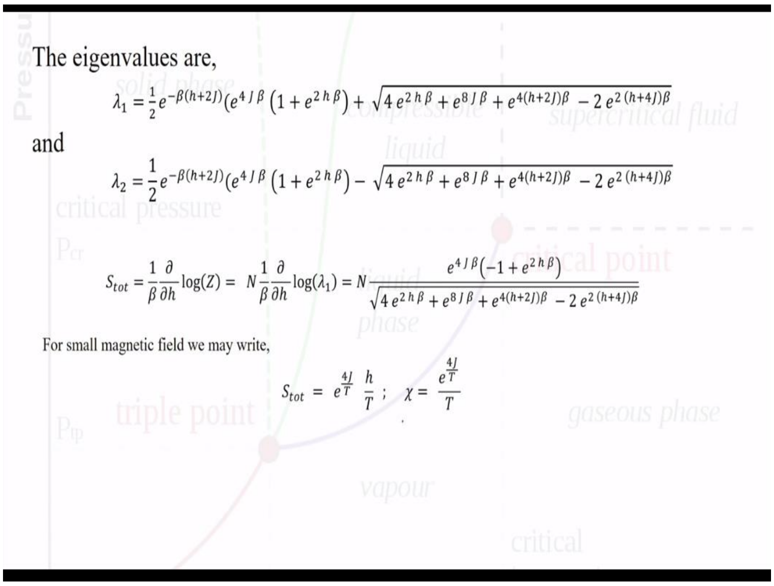

Okay so if you recall what we had stopped at the topic that we were discussing is the 1-D Ising model and we managed to convince ourselves that there is no ferromagnetic phase transition above absolute zero. That is because when we calculated the linear susceptibility, it remains finite for all temperatures except at absolute zero. So, indicating there is nothing interesting happening in the 1-D Ising model.

So, recall that this is the exact solution and so there is nothing you can do about it. So, that is how it is. So, as a result, the 1-D Ising model is a very uninteresting object. The only thing interesting about the 1-D Ising model is that it is exactly solvable, but then having solved it exactly, you find very uninteresting physics. So, strictly speaking we should be studying Ising model in higher dimension.

So, I promised that I was going to discuss the mean field or the approximate solution of the Ising model in higher dimensions, which does in fact show such an interesting phase transition, but before we do that I am going to just touch up on a topic which I ignored till now and that is the notion of spin-spin correlation.

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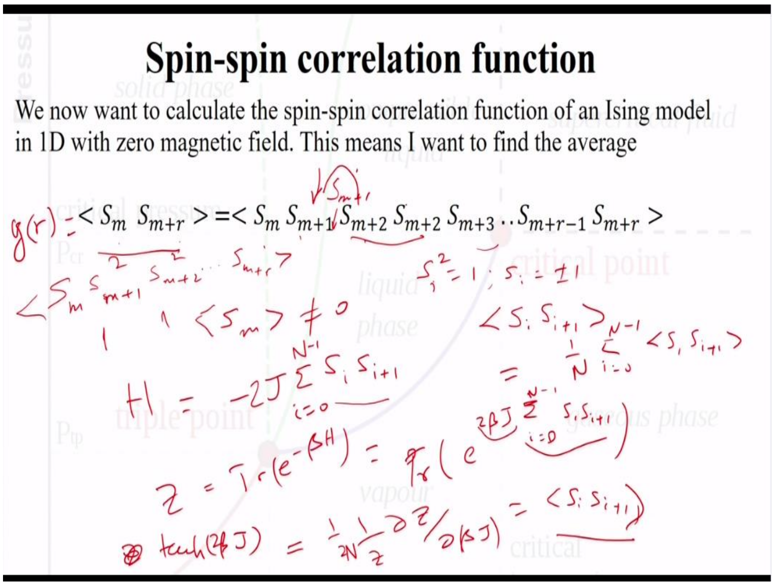

So, the idea is that in addition to well of course if you have a magnetic field, you expect the net spin, the average spin at a given site to be nonzero because the magnetic field is going to bias the system. So, that it is you know the probability that the spin is up or down, they will be different because of the magnetic field. So, as a result, the average will be proportional to the magnetic field and the proportionality is basically the susceptibility as we have seen.

However, in the absence of magnetic field, the net magnetic moment is 0 at least in the case when there is no ferromagnetism and so as a result that is an uninteresting quantity to calculate, but then you can ask yourself that in the zero magnetic field is there some interesting quantity that you can calculate with after all the average magnetization is 0. So, in that case, what is the interesting quantity that you can calculate?

So, it so happens that there still is an interesting quantity even at zero magnetic field that you can still calculate and that is what is known as the spin-spin correlation function and that tells you basically the spin-spin correlation is defined as the average of the spin at site m and spin at site r steps away from m, which is m + r. So, basically this is telling you that so the physical meaning of this quantity is that clearly it is a function of only r.

Because it is not going to depend on which site because recall that we have used periodic boundary conditions, so there is a translational symmetry that so at zero magnetic field is clearly going to depend only on r. So, what is the correlation between the spin at site m and spin at site m + r? So, depending upon how far away, how far apart m and m + r are, so you will get a correlation function which depends on r.

So, the interesting question to ask ourselves is how does this correlation function depend on r? So, in other words, how is the spin at site m correlated with the spin at site m + r. So, the answer to that the way you do that is to, well directly it is not possible to do this because recall that in the absence of magnetic field, so remember that we had decided that this is the, this is my Hamiltonian in the absence of magnetic field.

So, I can only calculate with some degree of ease this type of quantity, which is the correlation function of nearest neighbor. The reason why this is easy to calculate is because this is nothing but you can think of this $Z = Tr(e^{-\beta H})$, so which is nothing but $Z = Tr(e^{2\beta J\sum_{i=0}^{N-1} S_i S_{i+1}})$. So, given that this does not depend on i so this is 1/N times sorry this is 0.

So, this is nothing but i goes from 0 to N – 1 to S_i S_{i+1} and the average of this is clearly, so if I take

$$\frac{1}{2N}\frac{1}{Z}\frac{\partial Z}{\partial \beta J} = < S_i S_{i+1} >$$

okay so and then I divide by Z and then I divide by a further factor of 2 and then I divide by a further factor of N. So, that is going to be my average S_i S_{i+1}. So, basically that is what this is. So, if I differentiate with respect to this, I will pull this down and then I trace that over and I get this result.

So, it is easy to calculate this thing. So, now the question is how do you relate? So, what I want is not the correlation between nearest neighbors, I want correlation between m and m + r. So, the question is how do I do that? So, the way I do that is I start inserting yeah so I forgot to insert, there is an m + 1 there okay. So, remember that S_i^2 =1 because S_i is either + 1 or – 1.

So, S_i^2 =1, so if I insert, so I take S_m, so instead of I will put S_{m+1}^2 then I will put S_{m+2}^2, then all the way up to S_{m+r} will remain as it is, so but then that is what I have done. So, Sm squared is S_m, S_{m+1}, S_{m+2}, this is S_{m+2}^2, S_{m+3}^2 squared like that. So, I have not done anything great, I have just inserted a whole bunch of 1s here, 1, 1, 1.

But the advantage of doing this is because you see when I am called upon to evaluate an average such as this because of the nature of the Hamiltonian, which is quadratic in S. It stands to reason that this is going to decompose into pairs. So, it is up to me, how to pair up. So, for example, if I choose to pair up like this, so suppose I choose to pair up S_m and S_{m+1}, so let me go to the next page.

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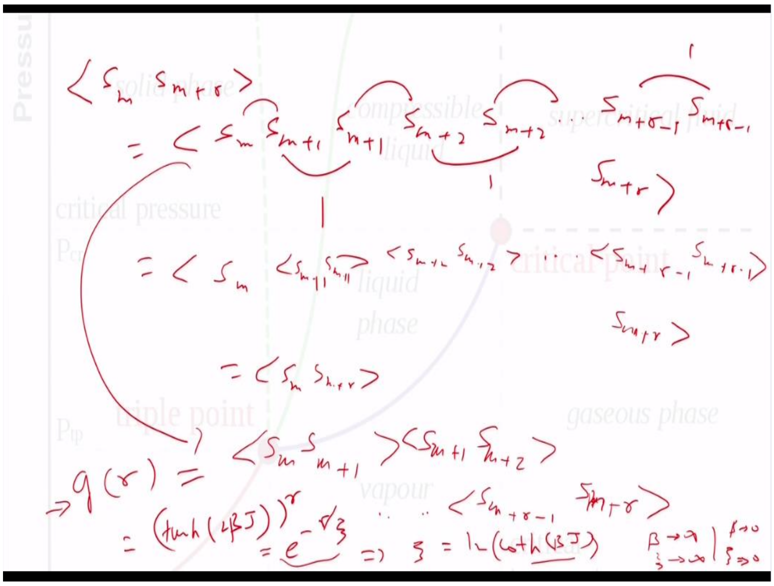

So, suppose I decided to do this okay, suppose I decide to do, S_m S_{m+1} S_{m+1} S_{m+2} S_{m+2} all the way up to S_{m+r-1} S_{m+r-1} then S_{m+r}. So, that is what I have just inserted 1 ,1 like that 1. So, now if I decide to pair up like this, I get back something uninteresting, I mean I can pair up S_{m+1} S_{m+1} and S_{m+2} S_{m+2}. So, if I decide to pair up like this, I get uninteresting result correct but uninteresting because I get back this for the same question.

I mean I get back the question I was asking. So, this is going to be S_m S_{m+r}. So, in other words, if I decide to pair up like this, so I can pair up any way I want. So, the useful way of pairing up clearly is to do this because if I do it this way, then I will be pairing up the nearest neighbors only. So, this is the useful way of pairing it up. So, now how do you calculate this? So, this is going to be my g(r).

So, the way to calculate this is to, so it is just to use this, this result namely, so this is going to work out to be if you just do this calculation, it is going to come out as 2 times sorry the 2 goes away and we are going to get $\tanh(2\beta J)$ that is what it is going to come out as okay sorry. Well, there is a factor of 2 which is missing. So, I am going to put 2 there, so it is going to come like that okay.

So, the answer is going to be $\tanh(2\beta J)$. So, now the g(r) is going to come out as

$$g(r) = (\tanh(2\beta J))^r$$

So, now it so happens that you can, so there is a standard definition of I mean there is a standard way of writing this correlation function. It is written in this fashion. So, this is called the correlation length. So, the idea is that you see the correlation between the spins at site m and site m + r.

They kind of it stands to reason that as you increase r, the correlation becomes smaller and smaller, that is because they go further and further apart. So, the nearest neighbors are correlated because of the J there and the next nearest neighbors are still correlated but be it indirectly because so say m and m + 2 are correlated because m is correlated with m + 1 and m + 1 is correlated with m + 2, so indirectly m is correlated with m + 2.

So, as a result, you can expect m and m + r to be correlated, although we expect that correlation to diminish rapidly and in fact not only we know exactly how it diminishes. So, the rapidity is described by an exponential decay. So, it diminishes as an exponential decay and in fact it so happens that you can write it like this. So, then you can end up writing the ξ which is the correlation length which comes out as.

So, you can write it in terms of the correlation length which is

$$\xi = \coth(\beta J)$$

So, this is the definition of the correlation length and so you can see that at very low temperatures, the correlation length is infinite. So, at very low temperature, when β -> ∞, ξ -> ∞ and when β -> 0 which is very high temperature, then the correlation length also become 0.

So, the idea is that so at very low temperatures, the spins are correlated over longer and longer distances. So, at very high temperatures set by the scale J of course at very high temperatures, the correlation lengths are very small, so that only the nearest neighbors are correlated. Although, this 1-D Ising model is very uninteresting, so as a result even the correlation functions are uninteresting.

But then the notion of a correlation function is important because when you apply to some more interesting models, it does exhibit very interesting behavior but not so in this example, this is well if you call this exponential decay interesting that is fine because that is that of course does carry some interesting information namely that the correlation decays are exponentially and the correlation length has an explicit formula in terms of temperature.

The uninteresting aspect to this is that, that dependence on temperature is uninteresting, namely it does not show any singular behavior at any given temperature beyond absolute zero okay. So, I am going to stop here as regards the exact transfer matrix solution of the Ising model.

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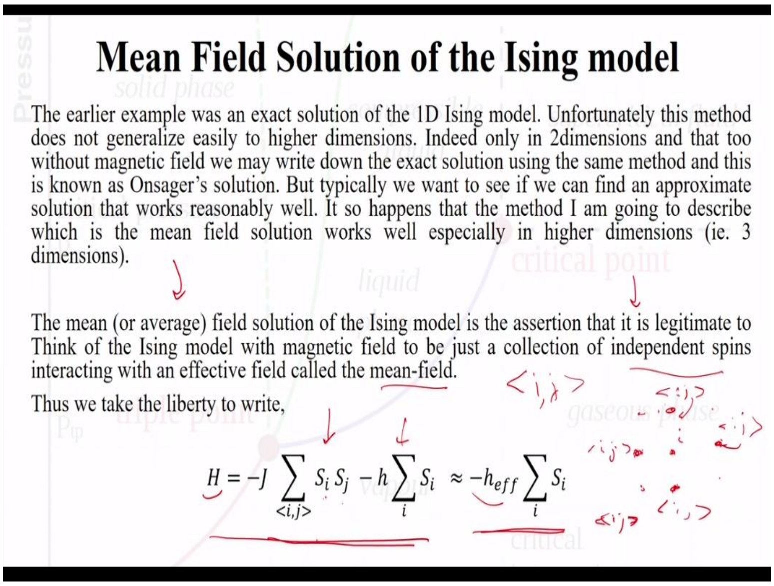

And then I am going to now jump to the mean field solution of the Ising model, which is of course going to be applicable in more than 1 dimension because in 1 dimension it gives you, we will see that why it is incorrect in 1 dimension. Then, as you go to higher and higher dimensions, it becomes more and more accurate. So, the idea of mean field is described in this paragraph here.

So, I am just going to read this out. So, the earlier example was an exact solution of the 1-D Ising model. So, unfortunately this method does not generalize easily to higher dimensions and indeed only in 2 dimensions and that too without the magnetic field, we may write down the exact solution using this transfer matrix method and that too with significant difficulty and that is known as the Onsager solution for the 2-D Ising model for which he won the Nobel Prize long ago.

So, it is a very difficult calculation and we are not going to describe that in this course, but then it is possible to do it but then it does not generalize to, you know systems where there is a magnetic field and certainly it does not generalize to 3 dimensions for example. So, for reasons that are little bit technical namely that, see if you notice that there was precisely 1 type of transfer matrix in the 1-D Ising model.

But then in the 2-D Ising model, there will be many more types and then unless they mutually commute with each other, the exact solution is not going to be possible and so happens that in the 2-D Ising model the different types of transfer matrices commute with each other so long as there is no magnetic field. So, that is the reason why it is exactly solvable. So, but then all is not lost because you can still invent an approximate method to study the Ising model in more than 1 dimension.

So, the way to do that is the mean field method. So, the idea of the mean field method like I have said here is that the mean or the average field solution of the Ising model is the assertion that it is legitimate to think of the Ising model with the magnetic field to be just a collection of independent spins interacting with an effective field called the mean field. So, in other words, so what is the picture that you have here?

You have a whole bunch of spins that are interacting with each other, but then you also have an external magnetic field. So, now the spins interact with each other and with an external magnetic field. So, the idea is now to replace the spins that interact with each other, so you turn off the interaction between the spins and then what you do is you replace the magnetic field by a certain effective magnetic field to compensate for the fact that you have turned off the interaction between the spins.

So, that new magnetic field or the effective magnetic field as it is called you have to calculate it self-consistently. So, how do you do that? So, you write down the Hamiltonian in this fashion and then you postulate that they should be writable in this fashion namely that the Ising model, so this notation, now remember we are not doing 1-D Ising model, we are doing Ising model in more than 1 dimension.

So, in more than 1 dimension, the i's and j's are on a lattice for example. So, the site i refers to the position on a certain lattice which could be a 2-dimensional lattice or a 3-dimensional lattice. So, when I talk of Ising model, I typically mean the nearest neighbor. So, if this is i, so <i,j> with pointy brackets I am talking about the nearest neighbor. So, then this if it is a square lattice and there are going to be 1, 2, 3, 4 nearest neighbors to this i.

So, this is one j here, there is another j there and there is the third j there and there is the fourth j there. So, all these are j's, the valid j. So, if you fix i, you are supposed to sum over the nearest neighbors to i. So, that is what this means, you fix i then you sum over the nearest neighbors of i and then you go to the next i and do the same thing and so on and so forth. So, that is what this means and you also have an applied magnetic field.

So, the idea is that put together, this can be approximated or written as an effective field times the total or the net spin. So, this is an approximation and it is not going to you know work always, specifically in one dimension it is not going to work at all alright. So, but in higher dimension, they expect it to work. So, let us go proceed thinking that we are studying higher dimensions.

And so how would you calculate for example the effective field. So, one way to calculate the effective field is just you know take the Hamiltonian and differentiate with respect to any one of the spins say that some particular spin, then clearly that is going to be your h_{eff}. So, now if I do that here, so effectively what I am doing is that I am differentiating with respect to S_k and then summing over all the nearest neighbors.

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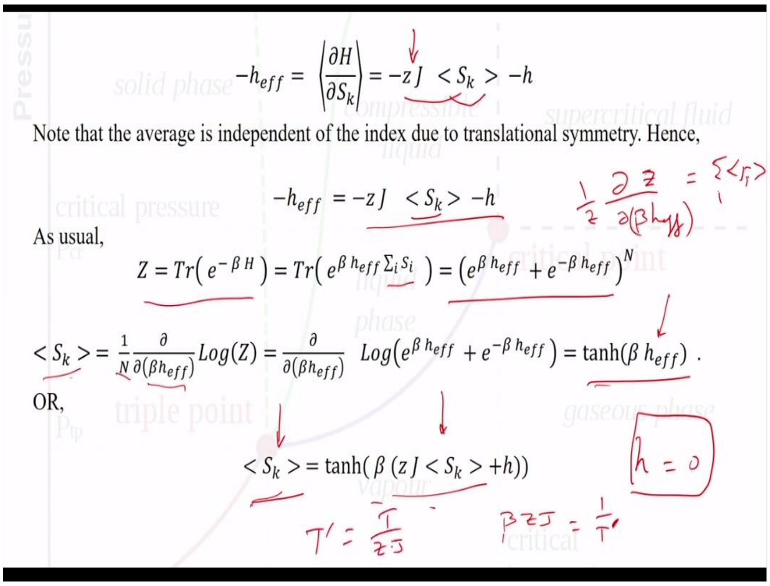

So, let us assume that there are z of those, z is called the coordination number, is the number of nearest neighbors to a given spin called S_k. So, it is how many nearest neighbors there are. So, that is how I am going to assume that there are z nearest thing, so the z nearest neighbors so I can write it in this fashion. So, this is h effective which can be written in this fashion. So, the average is now of course you know in this example because of translational symmetry, we expect the average because the magnetic field is uniform; it is the same at all sites.

So, we expect the average to be independent of k index. So, now so this is what we have obtained and now we can go ahead and calculate average of S_k independently as we normally do and so first we calculate the partition function and then you differentiate with respect to βh, so you get your total S sum over all the S's and then you divide by the total number of spins and that is your average of S_k.

So, I hope you get what I am saying. So, if you take the derivative with respect to you know βh_{eff}, so this is going to be S_i okay that is what it is. So, that is going to be this one okay. So, the point S is that the average S is going to be this and so as a result, I will be so remember that h_{eff} is going to be this. So, I can rewrite it in this fashion okay. So, this is called a self-consistent on a nonlinear equation for the average of S.

So, the unknown is average of S and it appears on both the left side as well as the right side. So, you will have to solve this nonlinear equation in order to determine the magnetization that is that the system possesses. So, it so happens that now there is some interesting physics going on here and that is described if you look. Clearly, if you switch on a magnetic field, you certainly expect a magnetization; you expect the average of S to be non-zero when there is a magnetic field.

But the really interesting question in this example is if is there a situation where if you turn off the magnetic field, if h is 0, is it going to be the case that there is still a spontaneous magnetization even without the magnetic field? So, that is the interesting question that we have to ask. So, in order to answer that we first decide to set h = 0 and then we plot the average spin at a given site.

I am going to plot it with respect to temperature. So, I am going to call βzJ, I am not going to call it anything, certainly it is some kind of a temperature. So, remember that $\beta = \frac{1}{T}$, so $T' = \frac{T}{zJ}$.

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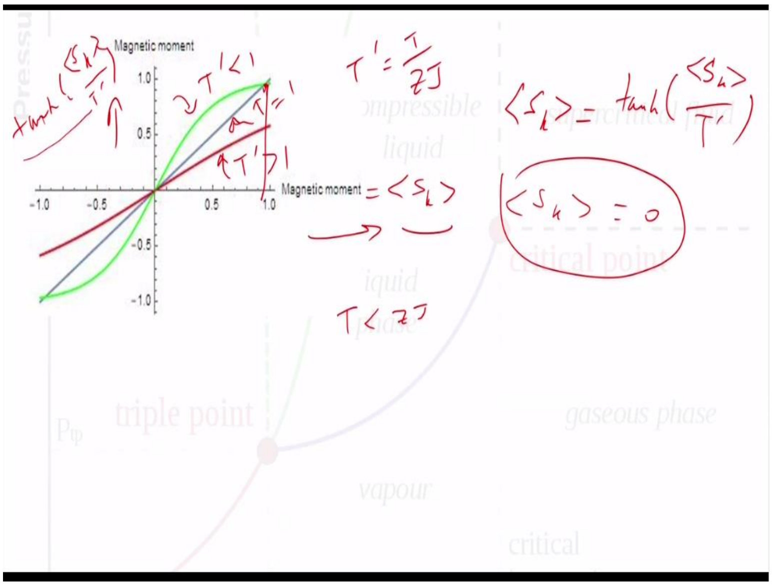

So, this is the idea that $T' = \frac{T}{zJ}$. So, when T, so the straight line is basically when T'is 1, so this is when T'< 1 and this is when T'> 1. So, this one is yeah so that is what this is. So, what are the x and y-axes? So, the x-axis is basically this one okay. So, this is basically average of S_k and here what I have plotted is tanh(<$_{Sk}$ >/T') you know.

Remember that h is 0, so it is basically tanh(<$_{Sk}$ >/T'), so that is what the y-axis is, so this is x. So, these two are equal, so basically average of Sk is equal to tan hyperbolic average of equal like this okay. Well, clearly one obvious solution is this is always a solution, that means all these curves pass through the origin, but that is not interesting. What is interesting is that the question is, is there a spontaneous magnetization that is possible?

So, the answer to that is very clear from this plot. So, if the temperature this T’ temperature if it is greater than 1 okay, so if it is greater than 1, it is not going to touch this. So, the question is when do these, this blue plot is just the straight line which is S = S. So, that is a reference. So, now the colored plots are the plot that I was talking about. The colored plot is this versus this that means tanh versus average of S.

So, those are the colored plots, the red plot and the green plot. So, now I have to ask myself where do the red plots and the green plots touch the straight line? Now, if you look at the red plot where the temperature T’> 1, so you see the red plot touches the straight line exactly at the uninteresting point namely S = 0. So, that means there is no spontaneous magnetization if the temperature is large compared to z J okay.

So, if it is the temperature larger than zJ, there is no chance of ferromagnetism. So, the average magnetization is 0. So, when temperature is less than zJ, you can see something interesting happening. So, the curve which is $\tanh(\langle S_k \rangle/T')$ vs $\langle S_k \rangle$, so that curve is going to touch the straight line at two interesting non-trivial points which correspond to spontaneous magnetization.

So, in other words, this is the value of the spontaneous magnetization that the system has. So, at any temperature, so if the temperature is less than zJ, so there is a spontaneous magnetization. So, that is an interesting prediction. So, it tells you that the mean field level, the Ising model in many dimensions, so that the coordination number is z. So, remember that in 1 dimension, the coordination number is 2 because there is the right side neighbor and the left side neighbor.

But then it is in higher dimensions like in 2-D square lattice, the coordination number can be 4 and so on or even more, it depends on the nature of the lattice, hexagonal lattice it could be more. So, point is that when the temperature is less than coordination number times J, there is a spontaneous magnetization and that is the prediction of the mean field solution of the 1-D Ising model.

So, it is an interesting non-trivial prediction and it is you can think of this model along with this approximate method of solving as a kind of a crude caricature or a cartoon of ferromagnetism in real materials. So, I am going to stop here. So, I have covered all the basics with respect to magnetism, I have discussed Landau diamagnetism, Pauli paramagnetism and then ferromagnetism as described by the Ising model.

So, in the next couple of lectures, I am going to see if I can discuss some slightly more advanced topics depending on how things proceed. So, I might cover topics such as renormalization group method of the Ising model, the solution of the Ising model and the method of second quantization for many particle quantum systems and so on and so forth. So, let us see we will play it by ear and see how it goes.

So, I hope you are enjoying these lectures and if you have any questions, please feel free to drop a line. So, see you next time.