Computational Physics
Dr. Apratim Chatterji
Dr. Prasenjit Ghosh
Department of Physics
Indian Institute of Science Education and Research, Pune

Lecture - 20
Monte Carlo Simulation Tutorial

Welcome back to the third class of this module on Ising model. So, in the last class what we did is basically look at the code how the flowchart is given, how the code was developed and now we shall basically learn to run the code and look at the data, the output of the runs. So, before actually looking at the data, the magnetization the average energy, the thermodynamic energy as a function of temperature one has to do various checks and cross checks to see; whether that the code which we are running that make sense with whether it gets a reasonable data, what is reasonable and we have also to discuss topics like when do we realize that the system has reached equilibrium.

So, we shall look at the data for different size of the lattices at different temperatures at instantaneous values of the energy and the magnetization as a function of Monte Carlo steps and we shall discuss the topics one by one ok.

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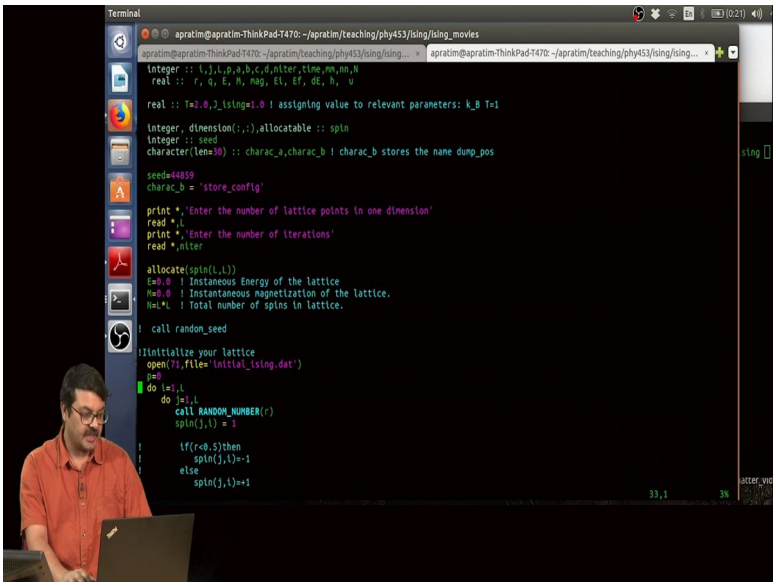

So, now this was the code that we discussed in the last class, now I want to just bring your attention that here over the entire lattice all the spins and the initial condition have been set to 1.

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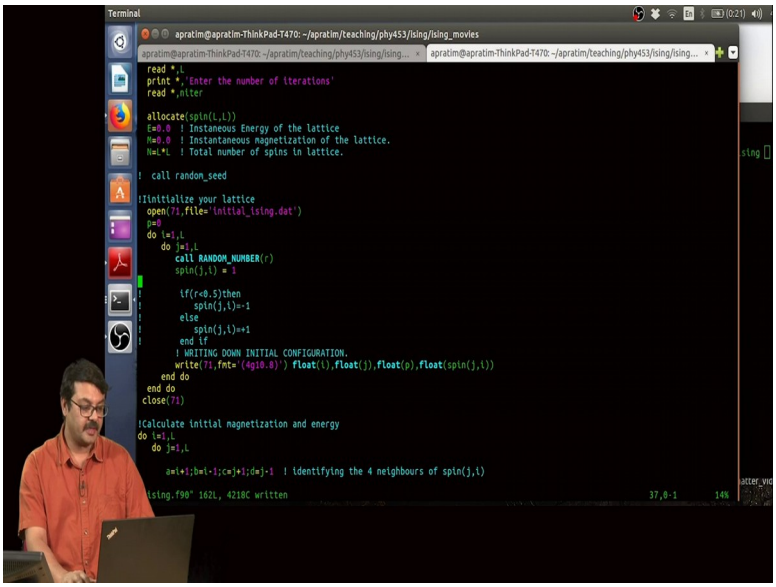

So, all spins are pointing up at the right at the beginning of the simulations the random configuration initial condition has been switched off which is in these lanes and let us see how we go about in running the data ok. So, I will be running the data, running the code at temperature 2 box size of L equal to 40 and initial configuration where all spins are pointing up ok.

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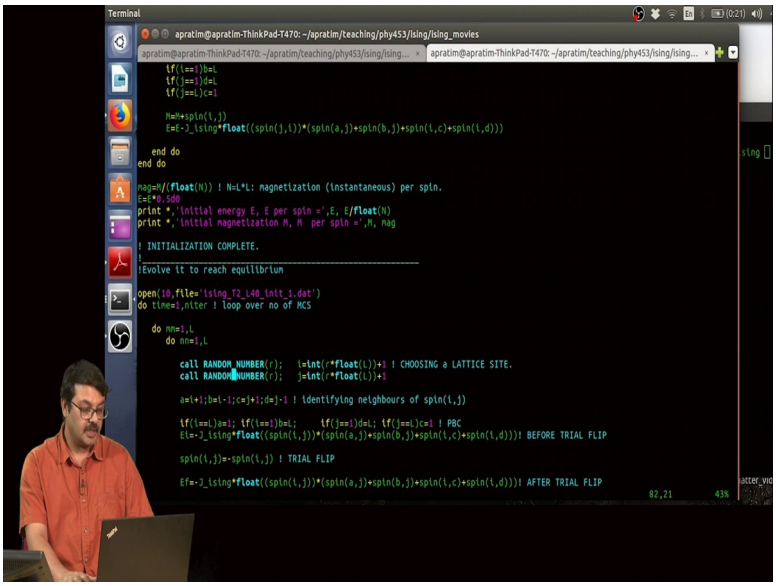

So, all the data which is basically number of Monte Carlo steps, the energy of each microstate and the magnetization per spin at each microstate will be saved in this file.

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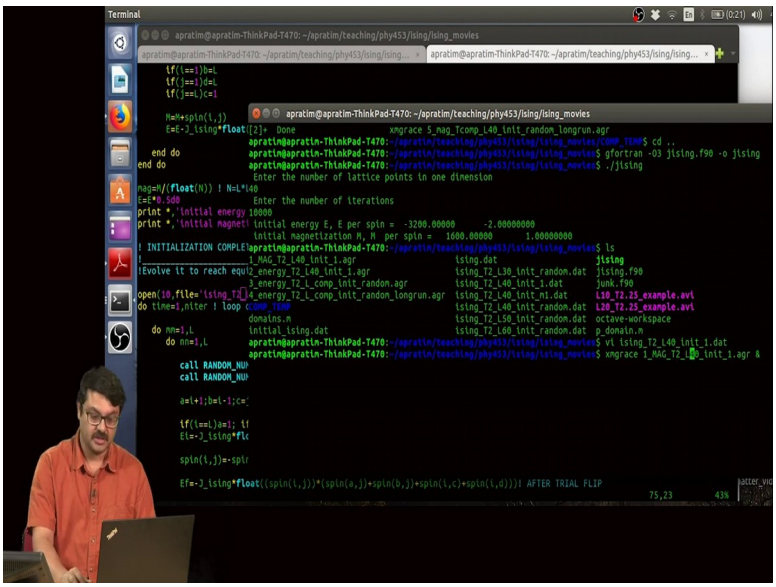

So, having told you that, so this file was called j ising dot f 90, I am going to compile it, so this is the command gfortran, you must have known this by now. So, I compile it and then I run it ok, I just type the name of the compiled file. It asked me number of lattice points in one dimension, which I shall give 40 and the number of iteration I shall give 10000 just as a

starting and the run is over just in 1 second. So, 10000 iteration, 40 cross, 40 lattice it takes around 1 second.

Here even before we look before we look at the data, note what is written here on the screen, the initial energy 40 cross 40 lattice is 3200, all spins were pointing up. So, the energy per spin was minus 2, which is basically written here minus 2 per spin and you have essentially 1600 spins into minus 2 is minus 3200. Initial magnetization all the spins are pointing up. So, the total instantaneous magnetization is 1600, there are 1600 spins and the initial instantaneous magnetization in that particular microstate is plus 1; this is basically M per spin. The data has been stored in basically ising T 2 L 40.

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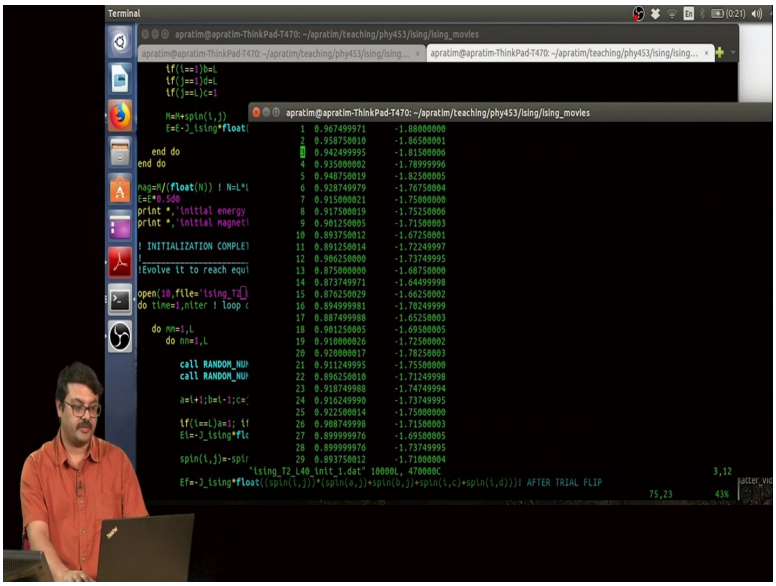

So, here is the number of Monte Carlo steps 1 2 3 4 it goes up to 10000; this goes up to 10000, the second column stores the magnetization per spin and this is the value of energy per spin. Now we are not going to look at the data 10000 of these data points, we are going to plot it ok. So, I have already plotted it and I am going to use the XM grace software to plot the magnetization per spin and we can use MATLAB new plot or whatever is a software of your choice to plot the data. So, here it is.

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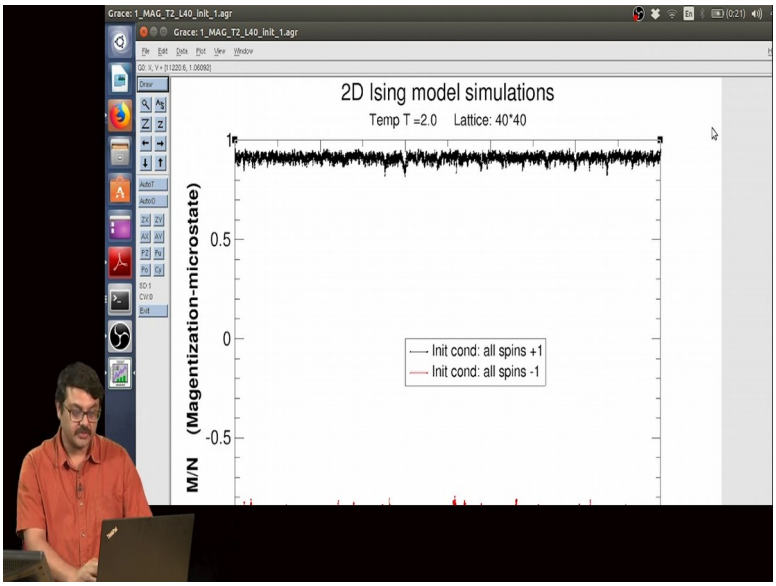

So, it shows that the magnetization at a temperature of 2 lattice size of 40 cross 40 is it started with all spins pointing up, but it is fluctuating around value of say around 0.9 ok, so this is basically the fluctuation. Now you can also start, where all the spins are pointing down. So, this is just the initial configuration.

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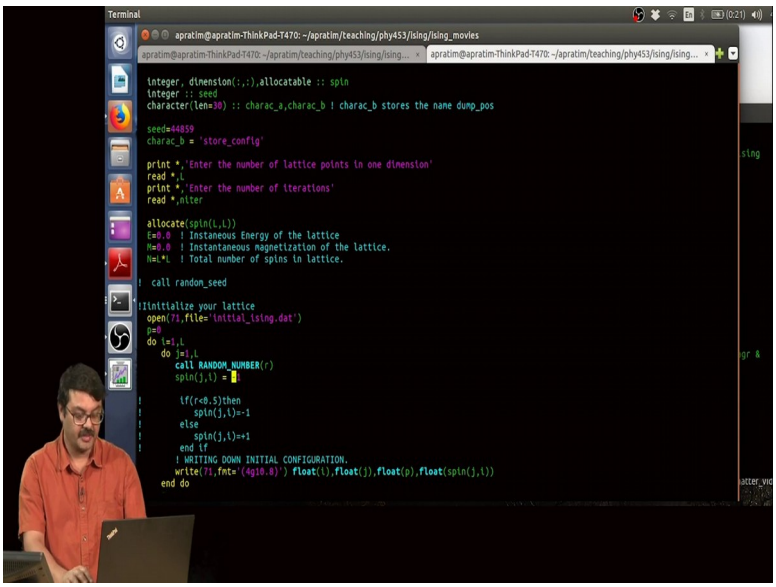

So, I just put this to be minus 1 all the spins are pointing down now, correspondingly I should save it in a different data file.

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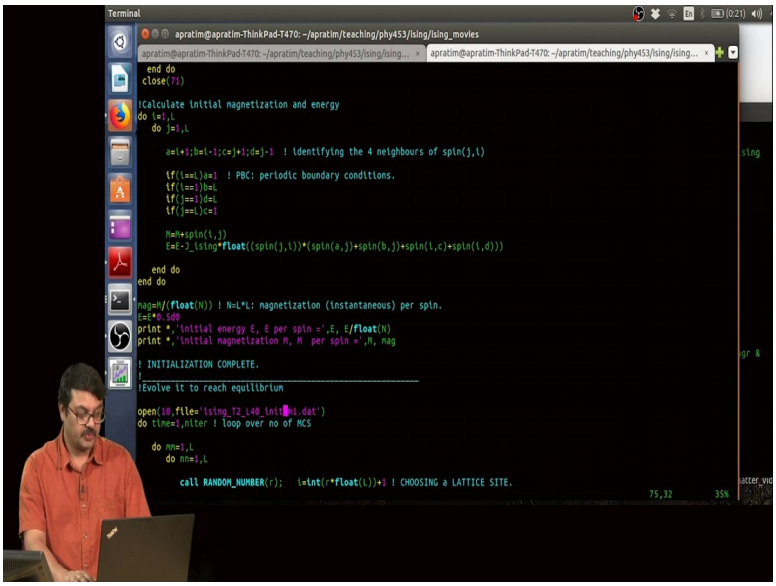

So, the temperature remains the same, the box size remains the same, but the initial condition I have said it is M 1 for minus 1.

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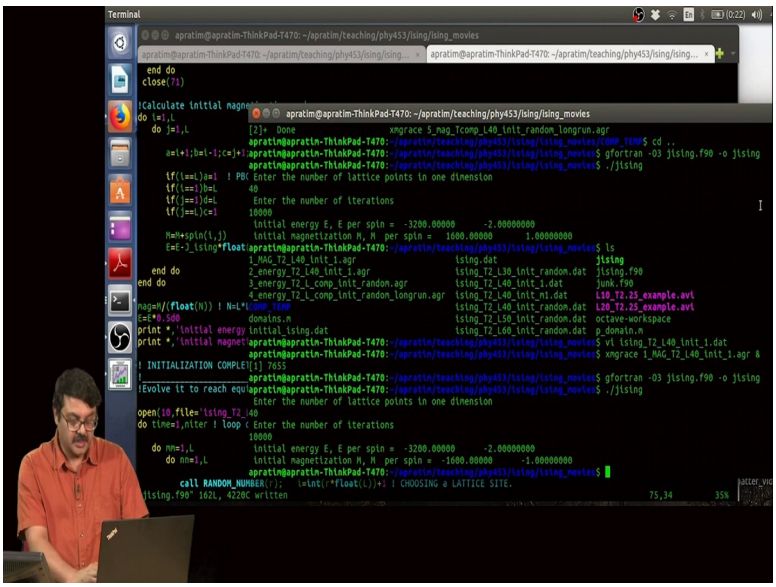

So, I again compile the code, because I have changed code then I run it. So, it is again 40, I want to run it for 10000 iterations and what I want you to point out to you that the total energy of the system remains minus 3200 as before.

So, all spins pointing up or all spins pointing down are identically the same that energy contribution is the same, energy per spin remains minus 2; but the magnetization now has

become negative right and the magnetization per spin is again negative, this is the initial condition.

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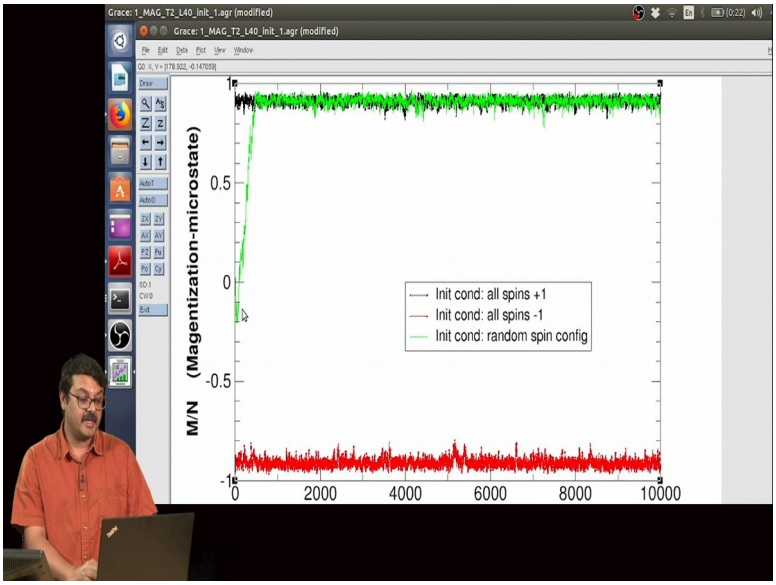

Now, if we look at the data and plot the magnetization, starting out from the initial conditions where all spins are minus 1 ok, it is this red graph. So, when we started out with the configuration where all spins were pointing up, then basically the magnetization per spin became around 0.9, it started fluctuating around 0.9 right; because why fluctuations because I am in each microstate there will be a different number of spins pointing up and down to the metropolis algorithm right.

You are flipping spin all the time and every trials spin flip, some flips are accepted some are rejected and the same thing is happening here yes; the magnetized the system is magnetized again, it has a magnetization which is fluctuating around minus 0.9.

So, all there are large number of spins which are now pointing down and a few pointing up; here the story is exactly the opposite most of them are pointing up and a few are pointing down, the magnetic state remains the same statistically, thermodynamically right. But suppose we started with a random initial condition, what would we get, should be something similar and I have already run the code and I am just plotting the data for you with the changed initial condition and that is this green graph. So, it is a bit different from the previous one.

So, this green graph is where the initial condition has been random spin configurations, right. So, half of the spins were pointing up and half of this spins are pointing down and. So, that is why it was around 0 the initial condition and it shows as you do number of Monte Carlo steps, it basically went and started fluctuating around 0.9. And that is exactly what we had discussed your value or your thermodynamic state, basically which consists of many microstates in equilibrium that will not depend upon your initial condition.

So, here it was plus 1 or it started from plus 1 and started fluctuating around 0.9, here it is minus 0.9; you might say that well you know the value of the magnetization is drastically different from plus 0.9 to minus 0.9. But the point remains that whether you call this up or this up right, it is a matter of convention the thermodynamic state is a large 90 percent of the spins pointing up or down predominantly, in a few pointing in the opposite direction. So, that determines the thermodynamic state of this system right; there is this up down symmetry in the system. So, it is equally possible that even when you start from the random initial condition, this data could have gone to minus 0.9 which would be in terms of equilibrium thermodynamic state it is equivalent.

But the choice of random numbers were such it happened, that it goes to plus 0.9 and starts fluctuating and you see that it is exactly I mean, statistically on top of this data. What is interesting is that, this data, this green data when you start from the random initial condition it takes around 1000 iterations, right for it to reach it is so called equilibrium value or rather fluctuate about its equilibrium average. So, you would say that this it is around 1000 iterations is the time that a 40 cross 40 lattice takes to equilibrate..

So, here we were looking at magnetization per spin and y axis is number of Monte Carlo steps; it is extremely important when you plot any graph to give the y label and the x label which basically define what you are plotting on your x axis and y axis, these are the legends. So, that you know that each of your data point, data set here green, red and black; what are the changes, what are they correspond to. So, here they basically correspond to different initial conditions, right.

Now, this we were looking at the magnetization per spin; let us look at what happens at energy per spin ok. I have again already plotted the data, so just then I have a look at what we have plotted.

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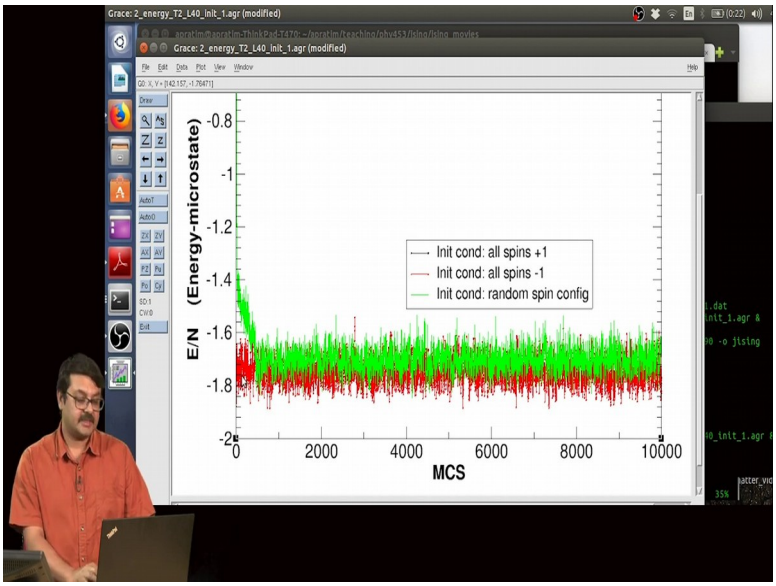

So, here this is basically data where we started from the initial configuration where all spins were pointing up; now I have already actually plotted the data for the other two cases. And the interesting point to note is, that the data where all spins are pointing in minus 1 right is exactly opposite to the initial condition where all spins were pointing in the up direction, that is exactly on top off. So, the red data where we started from all spins are pointing down and the black data where we all spins were pointing up there exactly on top of each other.

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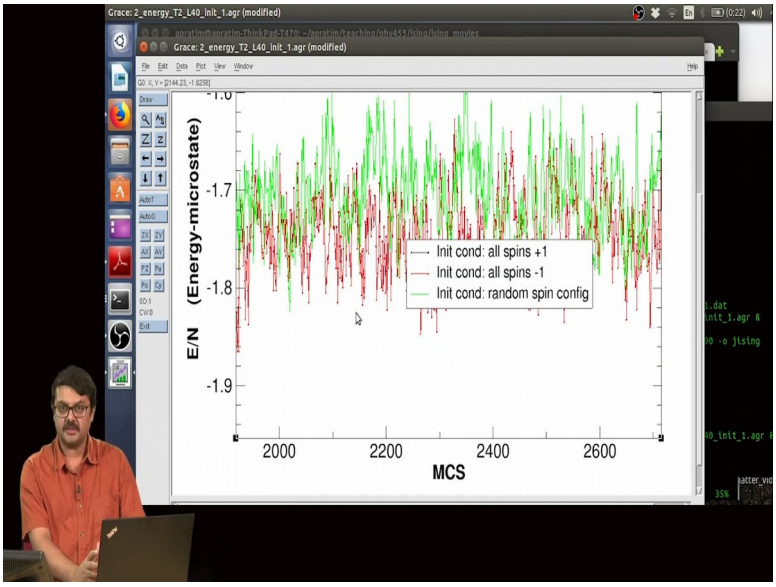

So, let us really look in greater detail and you see, you cannot basically figure out any difference between the red and black. So, why is this? The reason is basically whether you are starting from plus 1 or minus 1, right all spins up; you are generating the same random number sequence I did not change the random number seat, as a consequence you are generating exactly the same sequence of random number. So, whenever in the case, in the first case where all spins were pointing up, there were a few spins there were a few try trial spin flips which started, which were accepted and accepted to become minus 1.

When you start from all spins pointing in the negative direction, exactly the same spins are now being flipped up ok. Because the random number sequence is the same, even the choice the random choice of the spins which are being chosen for trial flips are the same. The other thing to point out is, when you start from random initial condition that is the sum of the spins are pointing up, half of the spins are pointing down which corresponds to this green curve; basically again it takes some time around 1000 iterations as we saw in the magnetization for it to reach equilibrium.

Now I would like to remind you, when we saw the magnetization data, the magnetization starting from out from two different initial conditions one went to plus 0.9 the other went to minus 0.9; but the energy of those configurations remain exactly the same and that is the reason why you are basically getting red on top of the black data, right ok.

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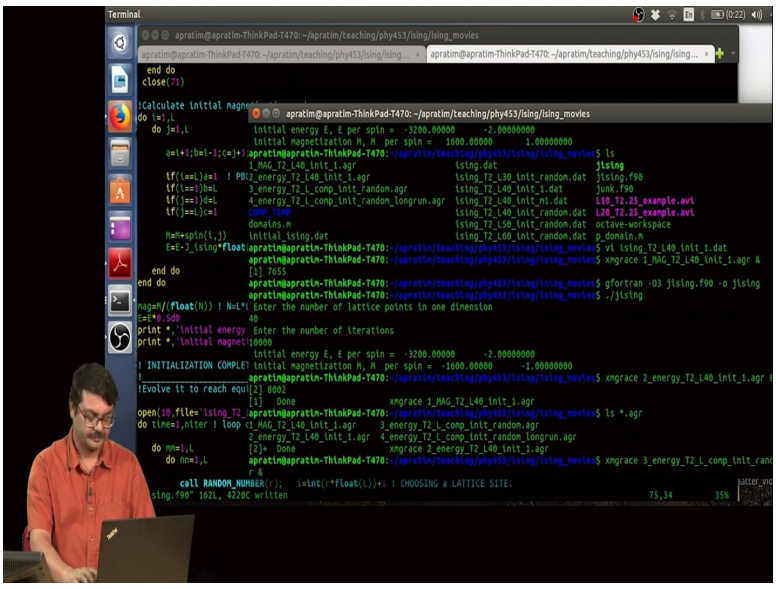

So, with this, just let us just move to the next step; now what would happen, right. Now, what would happen, if you took a slightly different size of the lattice , this was for box 40, 40 cross 40 and we started out from random initial conditions. So, the next question we are going to ask is basically we always start from random initial condition ok; where we see that it takes some time for the system to reach equilibrium state especially at temperature T equal to 2. And if we have different box sizes, then what is the kind of equilibration time we get and what is the quality of the data. So, I have already basically plotted the data for different box sizes, I have already run the code, I am going to just show you the data, right.

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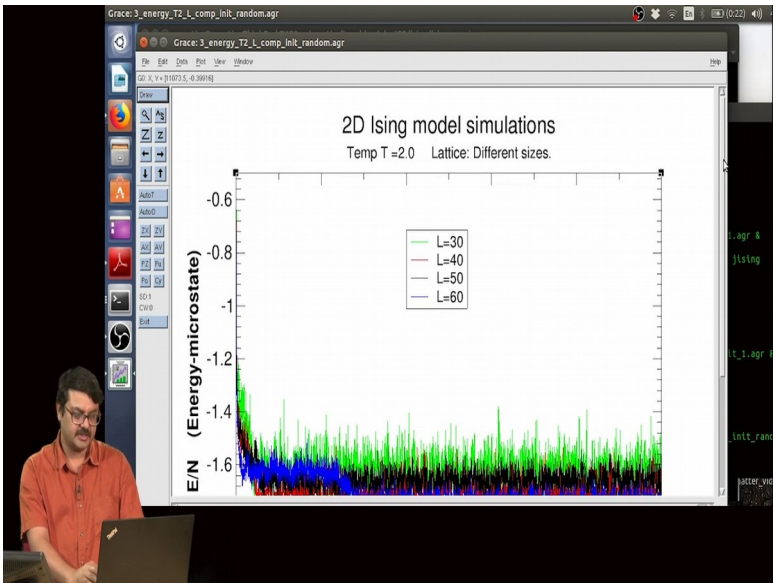

So, here basically we are again looking at 2 D Ising model simulations.

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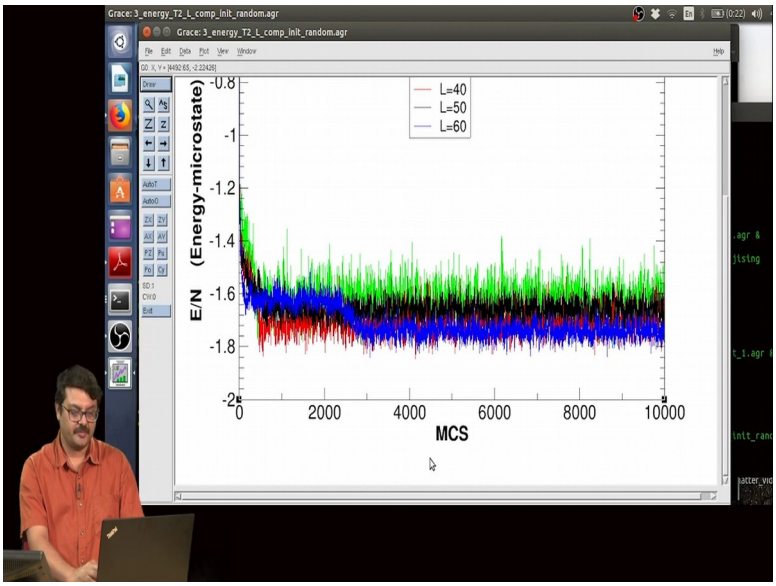

Where I am plotting energy per spin versus the number of Monte Carlo steps MCS and data is being plotted for L equal to 30. So, box size was 30 cross 30 and 40 cross 40, 50 cross 50 and 60 cross 60 right; temperature remains 2 and I am plotting data for different box sizes. So, you see the first fall, that the green data for L equal to 30, I mean the approximately are fluctuating about the same value, the energy is fluctuating around 1.6 and this blue one is a slightly less 1.7. The point is there is a slight shift in the energy; question is why? I mean you are talking about the same system, right.

On an average at temperature T equal to 2 an equal numbers of spins should be pointing up or down, I mean and it should not depend upon the lattice size; but there are lattice size artifacts and we will discuss this in future and we discussed that in the past. So, first of all this is the green data for the smallest box size and you see that for L equal to 40 which is this red data, so it basically equilibrates here. L equal to 60 there is a very sharp equilibration within whatever around 100 200 iterations; but then it gets stuck here and it finally, equilibrates here off it is takes around 2500 iterations. So, let us basically focus on this initial part in greater detail, right yes.

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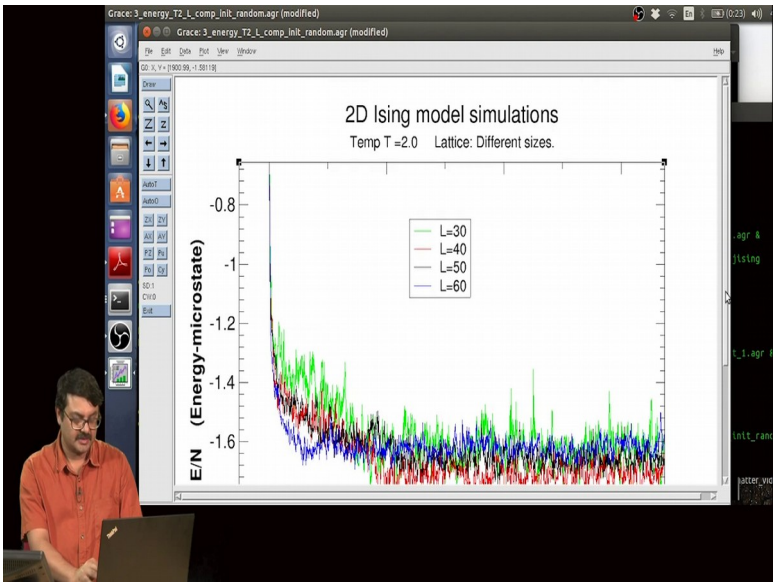

So, this is it. So, you see that for L equal to 30 it takes around 500 iterations before it reaches some value it starts fluctuating about an average after that; for L equal to 40 it states slightly more it is more than definitely more than the green data and so on for the black data which is for L equal to 50. And for blue it focuses, so for blue which is for L equal to 60 it rapidly decreases, starts fluctuating about an average; but then we know already from this that actually it reaches some equilibrium value at around 2500 after which at least up till 10000 iterations it does not seem to fluctuate much, right.

So, when we take data message, when we take data for equilibrium averages, thermodynamic averages which is what you measure in experiments that is exactly what you want to compare your simulation data with. You have to first figure out, what is the equilibration time for the blue data for L equal to 60 it is around 2500 after which it keeps on fluctuating at least April 10000 iteration and we should then check whether there is any further evolution of the mean. So, this is basically all of these data is fluctuating about the mean due to temperature all right, it is a canonical ensemble energy is fluctuating and it is fluctuating about a mean.

Whether there is any further shift in the data or not, only after we assure that the system has reached equilibrium; which means all these initial variations have gone and it keeps on fluctuating about an average value from that point onwards, in this case maybe like 10000 iterations forward ahead of 10000 iterations. We should basically check or collect data to calculate equilibrium averages and not before that.

So, here we see that there is a slight shift in the values of energies the question is why and let us check, if we run this data this runs for each box size for much longer number of iterations instead of 10000 MCS; suppose you run it for 100000 iterations, all right. So, do these data merge because do we seem to see some finite size effects, different box sizes are giving different mean values of the energy we have not explicitly calculated it, we will calculate it later; but you see that the fluctuation of this and the green is different.

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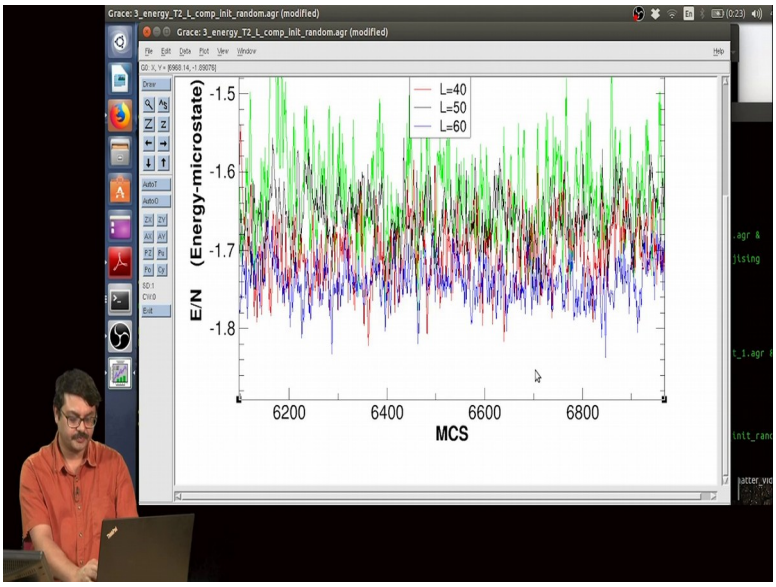

The other point I would like to point out that I would like you to note, that the fluctuation in this green data set for L equal to 30 the size of the fluctuation the magnitude of the, if you like the variance, if you calculated a variance and later you will calculate it. But even from I estimate it seems to be much more compared to the much bigger box size, which is L equal to 60 which is essentially 4 times bigger and if you take 30 cross 30 and compare it with 60 cross 60.

And that is not surprising, actually in statistical mechanics you know that the fluctuation goes as 1 by L right. So, or rather the relative fluctuations delta E, the standard deviation in fluctuations of energy by energy goes as 1 by root N; where N is the number of degrees of freedom is which is in this cases and 1 by root N would be basically N is L cross L. Having said that, let us look at the same data energy and magnetization for a much longer run, comparing across different box sizes and again I have already run that data for different box sizes for 100000 iterations, it takes around 3 4 seconds, it does not take much more than that.

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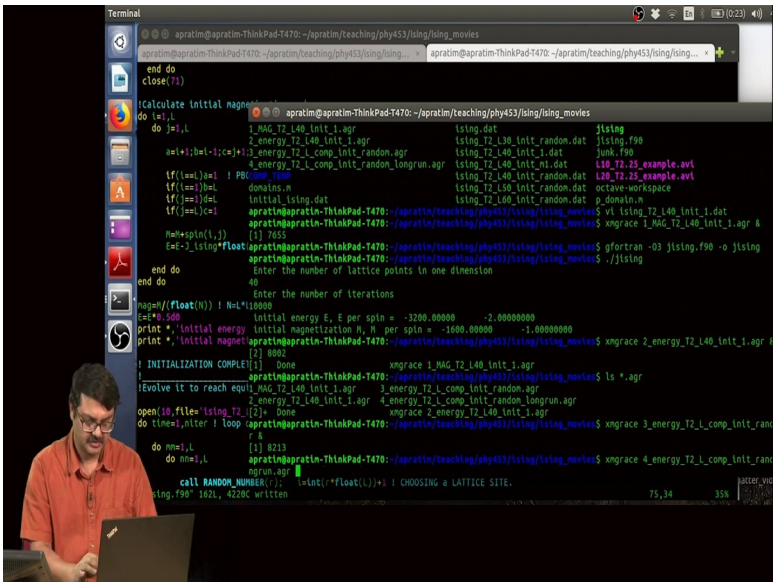

And if we look at the data, I am just plotting it for you ok.

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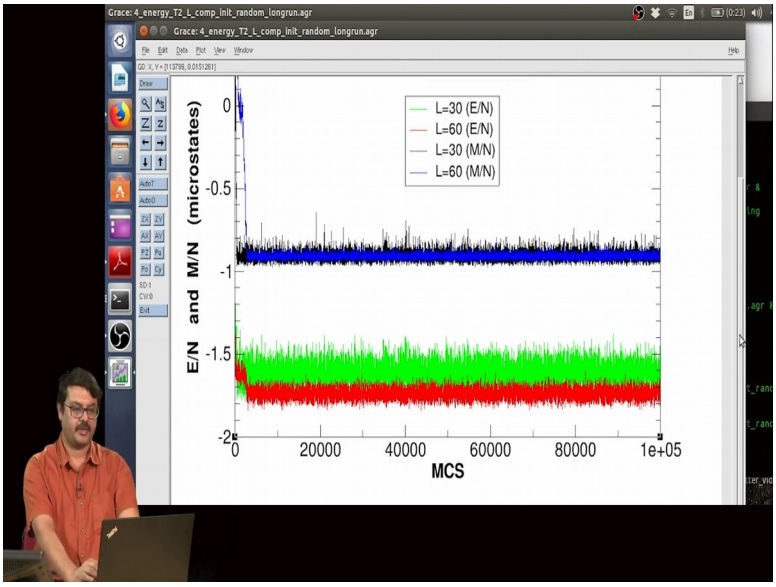

So, I have plotted both E by N and M by N for box size 30 and box size 60, right. For the energy we see that the green for L equal to 30 there is a distinct; so the fluctuation is about to mean up to 100000 iterations 100000 MCS is basically around 1.6. And definitely for a bigger lattice size L equal to 60 which is this red data, it is fluctuating around say 1.7 or 1.75. So, if we calculated the mean from this which would contribute, which would be essentially

the thermodynamic mean which you compare and this is all data at t equal to 2 then there would be shift.

So, which theta for should we rely on L equal to 60 or L equal to 30. This is another thing I would like to point out. Now if you look at the magnetization, but spend M by M this is E by N and this is M by N which I have plotted in black for L equal to 30 and in deep blue for L equal to 60. You see this is the initial, you have started from initial random configuration and it takes some time for the system to reach equilibrium and you see that the magnetization is exactly on top of each other, right.

The magnetization is around 0.9 or 0.95 and for the two cases it is exactly on top of each other; for the smaller box size which is this black, the fluctuations are more which you can understand from third from statistical mechanics. The variance does vary in thermodynamic quantities, the variance of thermodynamic quantities varies as 1 by N or the standard deviation relatives delta E by E or delta M by M varies as 1 by root N.

And that is exactly what we are seeing and you should actually calculate it the variance, for different box sizes and check whether it actually goes as 1 by N or not. So, the point is the magnetization is exactly on top of each other with larger fluctuations for L equal to 30; on the other hand low and behold that the energy has a shift wise that I mean, here it shows that an equal fraction of spins seem to be pointing up or down and here the energy corresponding energy is different.

The reason is, basically when you have L equal to 60 this is 4 times L equal to 60 is cross 6 as compared to a 30 cross 30 you have much larger domains ok. So, the average number of spins pointing up and down, rather the average fraction of spins pointing up and down remain the same; so fluctuation magnetization in is exactly on top of each other, the mean would be very close to each other.

But the size of the domains where some domains are plus and some domains are minus and there would be a domain wall in between the two domains. The number of spins which is sitting in a plus domain and the number of spins in between a plus domain and a minus domain, that would be more in L equal to 30, because the size of the domains is going to be smaller right; will later also show this in I shall explain that in the board also. But for L equal to 60 you have much larger domains; for L equal to 30 you have smaller domains and the

energy there is the energy cost for the domain wall and that is more for L equal to 30. If you have not understood it, we will discuss this later.

But it is clear that, before we start calculating thermodynamic averages we need to do a more detailed study of the finite size fx and that is exactly what we will be doing in the next class. But before that I would just end with showing you the values of the magnetization at different temperatures . So, how does it look like, so I have also again plotted that.

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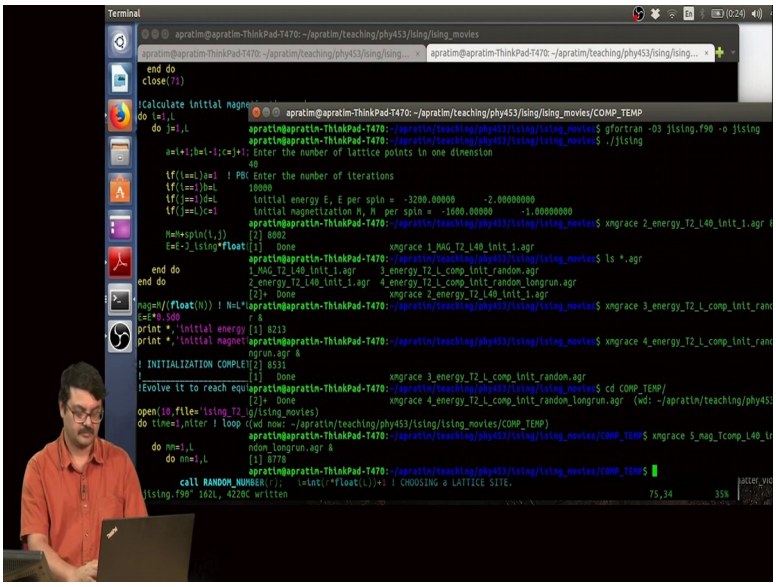

So, again I always start from random initial conditions.

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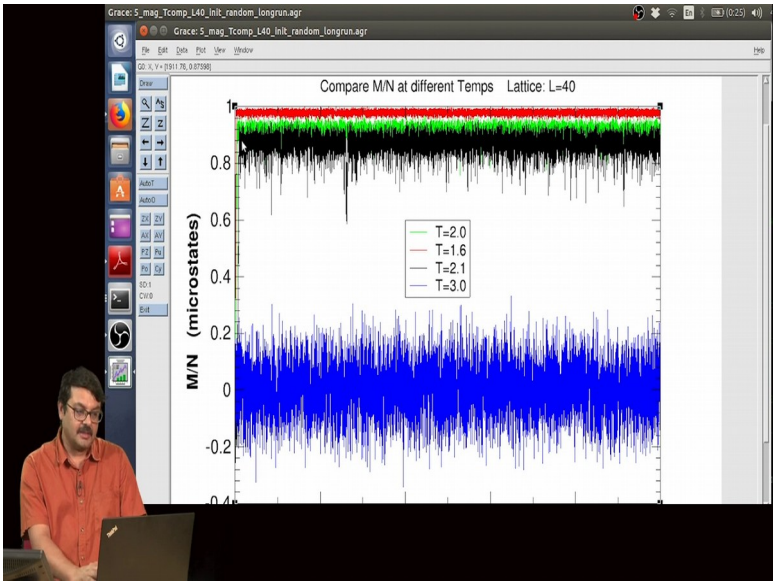

So, basically this is 2D Ising model where I am plotting the magnetization per spin, for at different temperatures, right, box size I have kept it fixed at L equal to 40. And basically you have already seen data for T equal to 2.0 and it is this green one and it fluctuates around 0.95. Now if I plot the average magnetization per spin that is at each microstate, instantaneous magnetization at for each microstate at 1.6; you see that it is even closer to 1, right.

So, you have a larger fraction of spins pointing up here, compared to that of temperature 2.0; that is not unexpected because at a lower temperature you have lower thermal fluctuations. So, the system is in a, so called more ordered state; I mean there are larger number of spins. So, more ordered by mean and the state is basically ordered, you have a larger fraction of spins which are pointing in the same direction; in this case the plus direction, right.

On the other hand if you increase the temperature, temperature T equal to 2.1, it basically fluctuates about a lower value. So, it is around it is whatever be the value it is around less than 0.9 this green being 0.9. So, now, it is fluctuating around a lower value and at temperature T equal to 3, it is fluctuating about 0; which means if you calculate the average magnetization you will get a 0 value.

So, this is a magnetized state at temperature 2, 1.6, 2.1 there is a magnetized state, you are getting a finite value of the magnetization it is fluctuating about an average value. But at T equal to 3 you see the magnetization has become 0; which means you have an equal number of spins pointing up and down and of course, that is fluctuating. So, the magnetized state is lost, the system is disordered right; you do not have you are basically gone above tc.

The other point I want you to note is that, at lower temperatures the fluctuation in the magnetization is smaller, you can absolutely calculate the variance once you have calculated the mean value. On the other hand, as you increase the temperature the variance the fluctuation is more. Again I ask you to refer, to your Stat Phyisics books and you would know that at higher temperature you would have larger fluctuations and that is exactly that you see here.

So, in the next class we will have a more detailed discussion of finite size effects and only after that shall we calculate the mean values of energy and magnetization and specific heat capacity and chi as a function of temperature; but that is for the next class.

Thank you.