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

Lecture – 23
Monte Carlo Simulation Analysis: Thermodynamic Quantities Part 01

Welcome back to the class. In the last class we discussed, how the instantaneous magnetization, the instantaneous energy varies as a function of Monte Carlo step at a fixed temperature, as we change different temperatures, different box sizes. And from that we realized that, if we average over different micro-states, if we average M or E over different micro-states and calculate this so called thermodynamic average of M or E; then and if we do it naively, then we could get wrong numbers. Because specially at small box sizes M could fluctuate widely from plus M to minus M and if you average it naively you will might get a 0 value of average M; whereas, actually the system might be magnetized.

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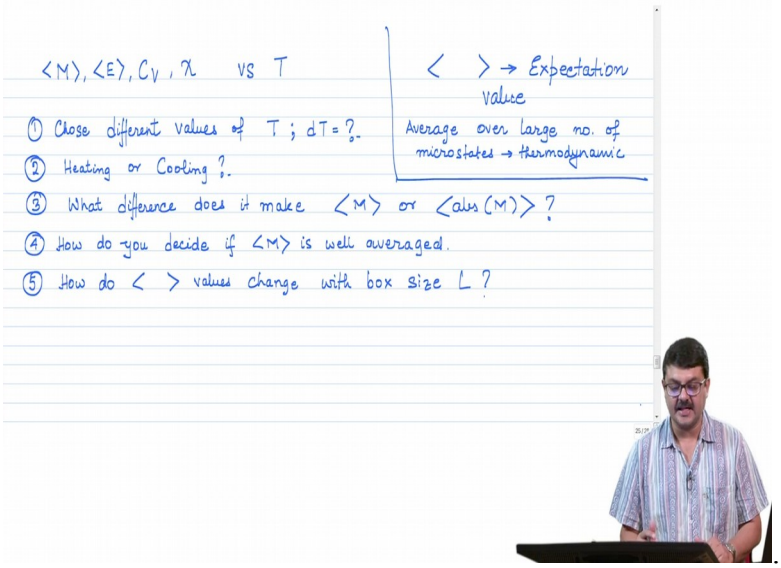

With this background that we discussed last class, what we are going to do today is systematically look at calculation of average M, average E, C v and chi versus temperature. So, here I have put in angular brackets and angular brackets essentially mean, it is an expectation value it is an average value, average over different microstates;

that is the thermodynamic average. When you have basically averaged the value of M i instantaneous magnetization and averaged the value over different micro-states simply added it up and divided by the total number of micro-states access. Then you get the, so called thermodynamic value which is the quantity which you measure in the lab or which is the quantity which you calculate using your statistical mechanics, right.

Now, even as we plot these quantities versus temperature, there are various questions that immediately arise when you are doing simulations. Of course we are going to calculate these quantities at different values of temperature and how closely should be very temperatures.

So, what should be the value of d t? So, like suppose 3.1, 3, 2.9 or should it be smaller values of d t weight 3, 2.95; so what how much should be the change in temperature, how much should we wait before the system reaches equilibrium? We already discussed about relaxation times in the previous lecture; especially I would ask you to note that at lower temperatures the relaxation time, the time that a system takes to reach equilibrium at that particular temperature might increase. So, at low temperatures, you typically have larger relaxation times, right.

When we are plotting these quantities, in various thermodynamic quantities should we take the heating curve or the cooling curve? Ideally if it is a system is perfectly equilibrium in as per equilibrium statistical mechanics we read in theory, they should be identical unless there is some hysteresis. Hysteresis is there in first order phase transitions, this one we that we are studying is 2nd order phase transition, so ideally there should be no hysteresis. But often there are problems, but are we getting identical curves during heating or cooling; these are things to check before even you start to plot analyze your data or and start drawing conclusions.

We discussed this aspect later, what difference would it make in the phase diagram. If we use average magnetization, if we calculate the expectation value of magnetization or if we take the absolute value of M; so that both positive or negative values of magnetic states basically have some finite value of M and then we average over that. What difference would it make? We already discussed we are going to use this to calculate our phase diagram. In the phase diagram on the y axis, one shall have the thermodynamic value of the order parameter, which in this case is the magnetization.

On the x axis there shall be temperature and shall plot in the phase diagram; how does magnetization change as a function of temperature and at what value of temperature does the magnetization become 0. Basically we have the transition, the phase transition from a low temperature ordered phase to a high temperature disordered phase; where the system essentially becomes in the paramagnetic state, in the paramagnetic phase, right.

How do we determine this temperature accurately? Does it depend upon the box size, I mean ideally it should not, I mean in typically in physics you are discussing about N equal to infinity, N being the number of spins, right, so you have a fixed temperature. But in simulations, we are doing simulation with suppose a 20 cross 20 box or a 40 cross 40 box. So, which means you have 400 spins or if you have a 40 cross 40 box we have 1600 spins, does that give the thermodynamic limit; how do we get the thermodynamic limit, right; I mean we were which should match with experiments, is there some finances effects or not.

Other question is, how do we decide, at any particular temperature over how many Monte Carlo steps should we average, so that we can claim that the expectation value of M is well averaged? Right. So, these are the questions we shall be discussing, debating, trying to figure out even as we plot various thermodynamic quantities to identify the transition temperature; and basically to see and to see or to understand the phase transition.

So, with this background, let us basically move to the computer and start looking at graphs and data, which we have generated; which I have already generated for you using different runs where we where I save data at different temperatures, different box sizes, heating or cooling in different files by changing the files which is basically done here.

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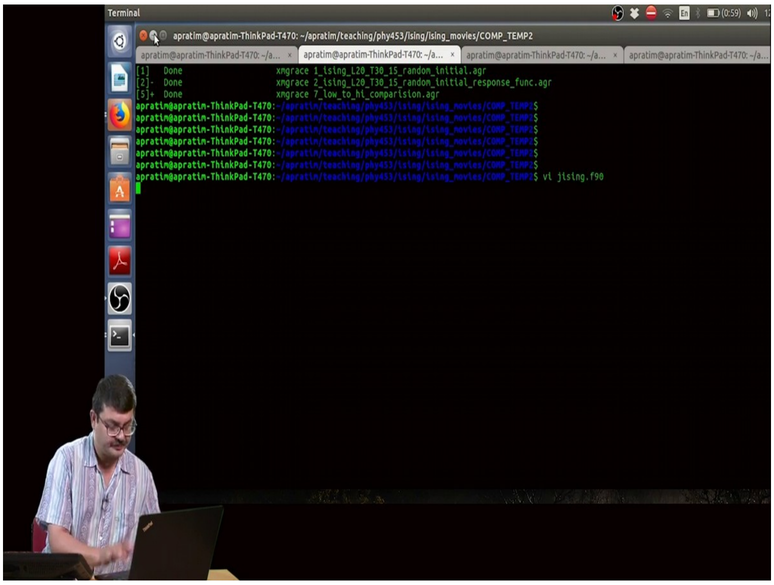

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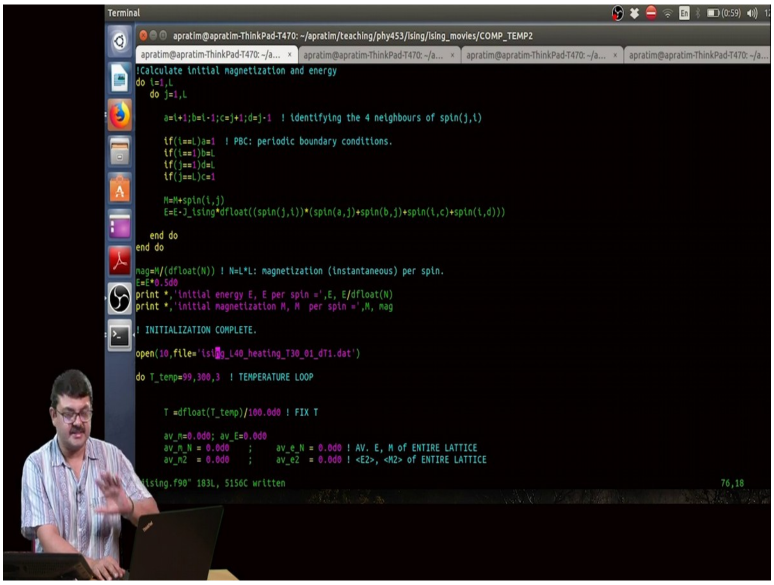

So, as I change the conditions, as I change the box size, as I changed the values of d t, I have been changing these name of the file; this is the same code that we discussed last time suitably modified, so that we can look at averaged quantities with temperature. And you have to give different names as you do different runs and plot them together to compare different cases right; we shall do that, you shall see that.

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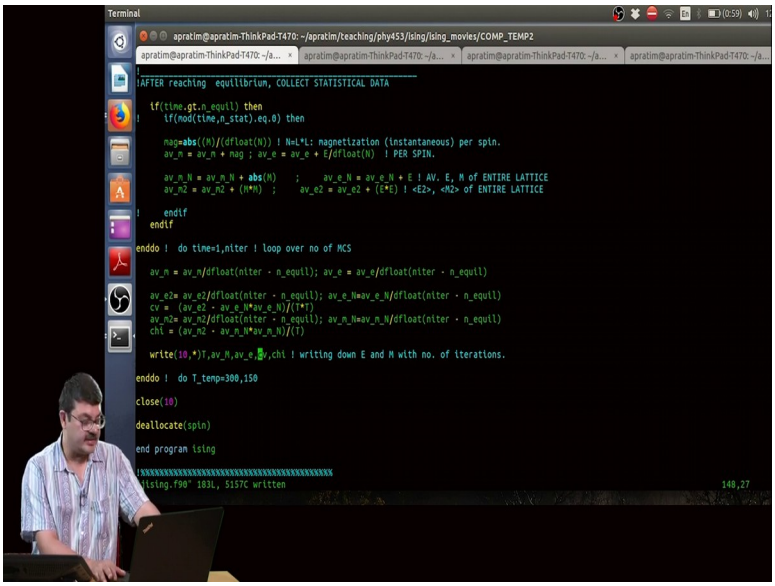

The other thing I insist on reminding you is, when I plot the data to compare across different box sizes, I shall be plotting magnetization, average magnetization and average energy per spin, right. And that will be calculated here, basically abs absolute value of M and sometimes I also remove this absolute value; so that I can compare the magnetization, the average magnetization when the absolute value is not taken, right.

So, here I have divided by d float N; N is the total number of spins. So, basically I have magnetization, in this step I am calculating the average magnetization per spin right; and similarly I am calculating the average energy per spin. But when I want to calculate C v or chi, the specific heat capacity or the susceptibility I do not divide it by N; I want the fluctuation the e square minus e average square or m square average minus m average square of the entire system .

So, I do not divide it by N, I want to look at the fluctuations of the entire system, the heat capacity of the entire system, right. And that is what I will be plotting and here I have not divided by d float N; here I am calculating the average magnetization of the entire box, different box sizes for different fronts. Here I am calculating M square for the entire box right and here basically, so after this at each temperature after nitter iterations, which I shall choose to be 100000 . Then, so basically I shall choose nitter to be 110000 because at each temperature I am going to discard the first 10000 Monte Carlo steps, because I

will allow it to equilibrate the new temperature for 10000 steps and then I shall calculate the average value over the next 100000 or 10 to the power of 5 iterations, right.

So, here I have given an if statement, if time is greater than n equal then only start collecting data for thermodynamic averaging. And after this loop is over, I am basically calculating the average value averaged over 'nitter' minus n equal number of iterations right. And then writing it down enough in a file where I am writing down temperature, average magnetization, average energy C v of the entire box, the specific heat capacity of the entire box and the susceptibility. So, this there will be 5 columns and I shall be plotting it for different box sizes, right.

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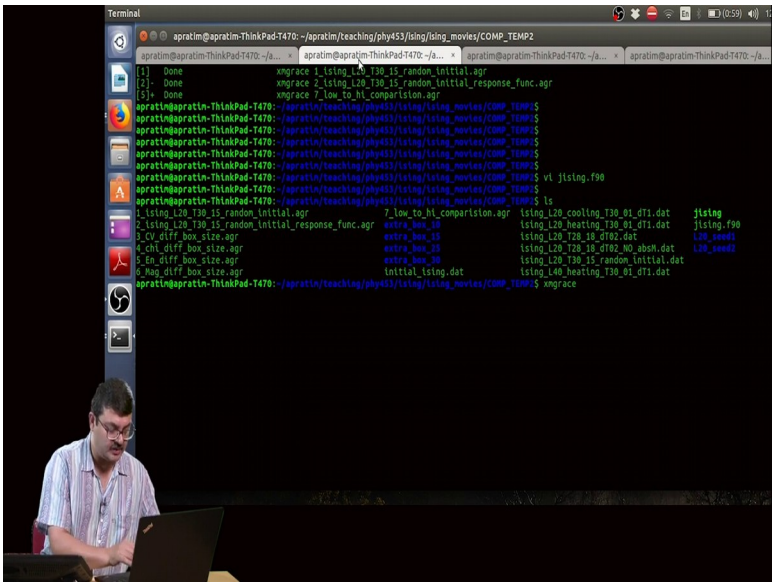

So, I have already done that and so, just for the sake of completeness, I shall compile it once again for you. And now I shall run it, the box size is 20 cross 20 and the number of iterations at each temperature is 110000, 10000; 10000 iterations are you are giving it to equilibrate. And it is going to run for some time, it is going to take around a minute; and then, but I have already done this and plotted data. So, let us now look at the analysis of data.

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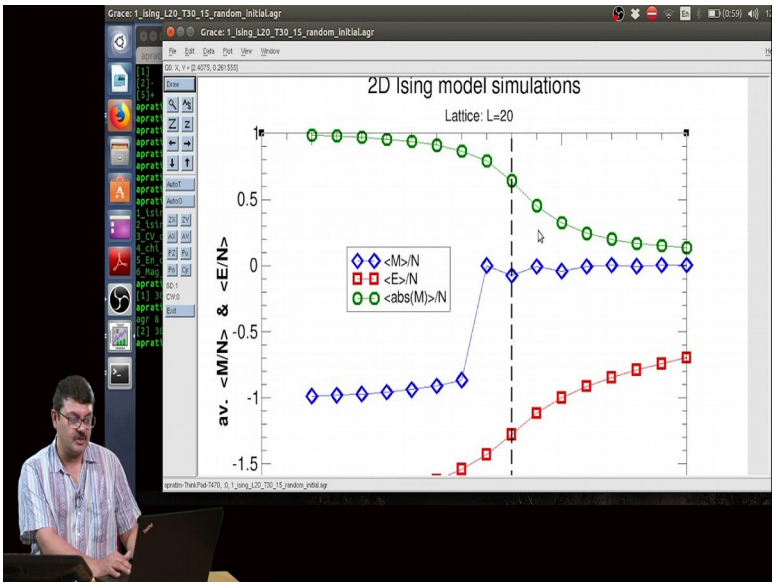

So, what we see here is essentially the average magnetization and energy. So, this blued data is the magnetization versus temperature, the on x axis I have a plotted temperature, dt has been 0.1 the box size is L equal to 20. And what I have plotted here, is the average magnetization where I have not taken the absolute value; and this green data is where I have averaged by taking the absolute value of M.

So, whether the state of the system is positive or negative. So, all spins pointing up, most spins pointing up or down. If you take the absolute in value of the instantaneous magnetization right; then you will always get a positive value independent of whether value of instantaneous M is positive or negative. And I had to do that, because for specially for small box sizes you might end up getting a wrong value. We discussed this last class, if you have any confusions please look back at the last class.

And what we see here, in the data is when you plot expectation value of M doubt the taking the absolute value at higher temperatures, you get 0 value as expected; because sometimes the spins are positive, sometimes the spins are the average instantaneous magnetization is negative and it is fluctuating about the 0. And you when you take a good average it should be 0, but at a temperature of 2.1 it suddenly jumps to minus 1, which means there has been a transition here all right; but this shows up as a jump.

Now, knowing about ferromagnetic transitions, we already know that this is a 2nd order transition and the data should look more like this where it is gradually increasing from 0

value to a finite value and not a jump; a jump is indicative of a first order phase transition.

Now, in this case we already know, that there is a problem because we know about the Ising model, one can has analyzed it over many years. But it is important that, suppose you did not know whether a phase transition a first order and 2nd order, then how would we approach the problem right. So, we will discuss all these things. So, here it shows a jump, but we know that this calculation is not appropriate, we would rather use the absolute value of M to calculate it and that shows a gradual increase as it should.

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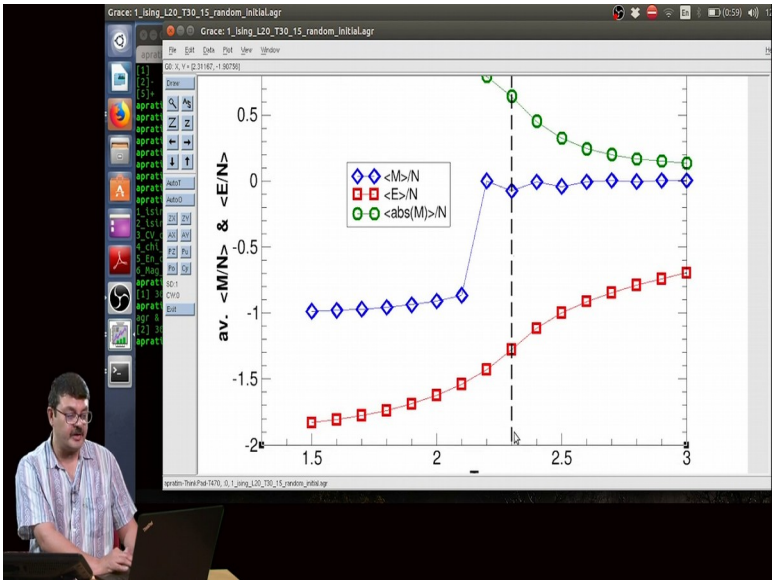

But if you take this absolute value the artifact that you are introducing into the system is above the transition which is just below 2.3; I have drawn this dashed line just as a indication that transition should have happened. It is already known that the transition should happen here, actually slightly less than 2.3 I have drawn the line exactly at 2.3; so here the transition, so at 2.3 the magnetization ideally should be 0.

But here we see a finite value moreover and even higher temperatures you do not get 0 magnetization as you ideally should get, as you get here; but here you are getting a finite value that is because even the fluctuation sometimes positive, negative it is always taking the positive value. So, this is the error that you are introducing into the system, here it is definitely showing a wrong value, that this is magnetized. It shows that there is no

magnetization here; whereas, we know that the magnetization actually occurs at some such value, at a value of around just below 2.3 as I said at some such value right.

So, here it is showing a wrong value, because of large scale fluctuations which happens near T c; and even from here, from this data for L equal to 20 we cannot exactly identify what is the transition temperature. Questions is, should we look at the data of C v and chi which is suppose to show a peak, from there can we extract this value. Now, the question is, should we plot this data with smaller values of d t; so that you have more finer points between say even a change of d t equal to 0.1.

Here this is the data for energy, energy per particle it basically at higher temperatures it has a value close to around minus 0.5; but as you lower the temperature so, there is a change here and it gradually goes to some number close to minus 2. Here I have changed, taken the range of temperature to be 1.5 to 3; of course, you can take your system down to lower temperature we will do it at a later point of time. But here we at the moment our focus is, trying to identify the transition temperature .

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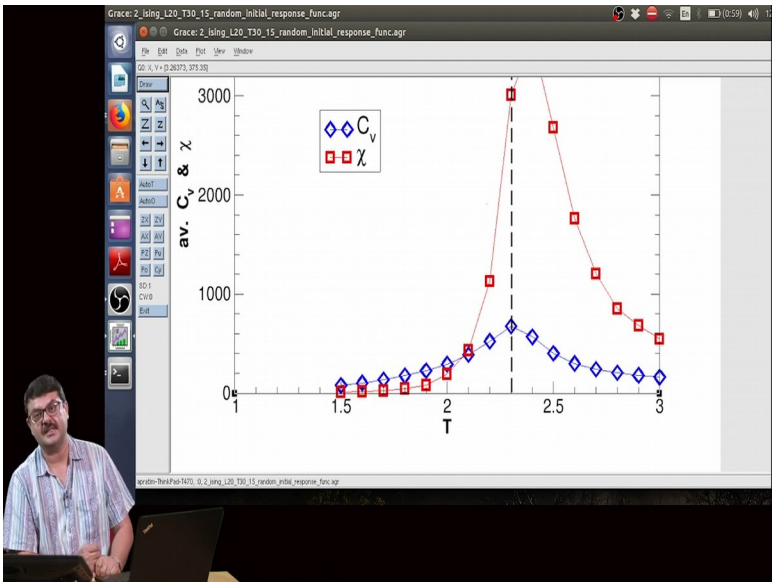

Now, we saw from the data of M or and E that it is difficult to identify what is the transition temperature. So, in this plot I have plotted average C v the e square average minus e average square by t square and chi m square average minus m average square by t k B is 1; and the basically the red curve shows chi, the blue curve shows C v. And I have plotted this versus temperature it is extremely important to always give access

labels, the figure should be easily seen and readable, just like I hope it is easy for you to see. And this is for lattice size of 20, I have labeled it properly; this is the way to present data, when you show it to anybody including in your exams anyway.

But focusing on the data, we see that there is a peak in chi at around 2.4 and there is a peak in C v at 2.3. We also notice that it is possible that the transition could be somewhere here or here and definitely the value of d t might not be good enough. Maybe we should have smaller values of d t, so that we can look at identify the temperature at which the transition happens more accurately.

This discreteness is not sufficient for basically identifying the transition temperature, because it could be anywhere in between these two values; and moreover these two the peak, the position of the peaks are not matching. Is there a dependence on L? What if you plot the same quantities for different box sizes? Let us have a look.

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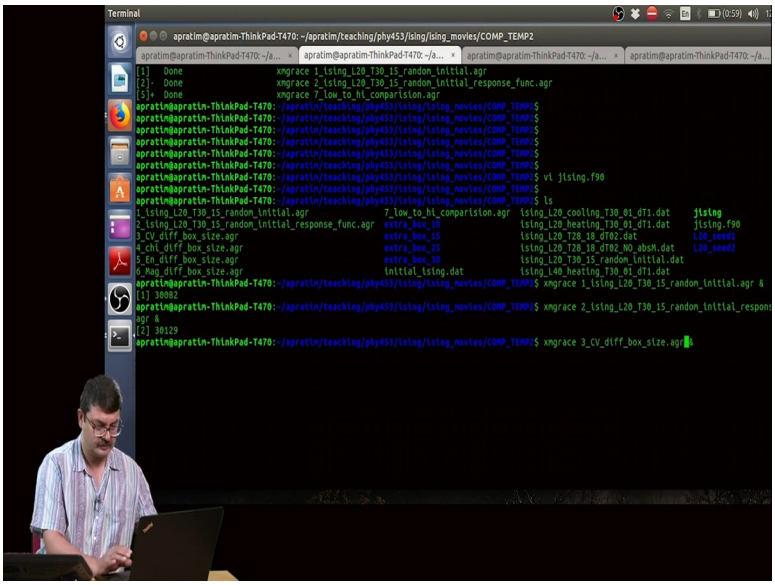

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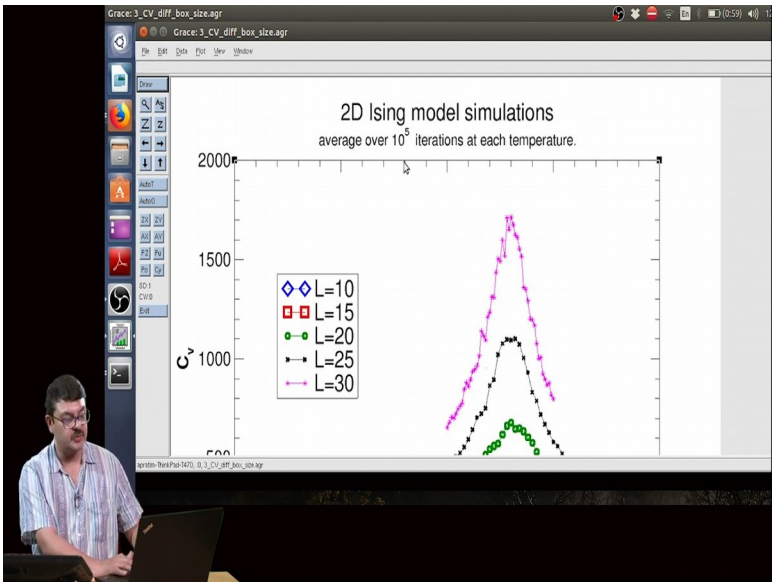

What I have done here is plotted C v , the specific heat capacity for different box sizes L equal to 10, 15, 20, 25, 30 right. At each temperature to calculate each of these points, basically I have averaged over 10 to the power 5 iterations at each temperature; and then I have varied the temperature allowed the system to reach equilibrium at that temperature. And then averaged and calculated the average value of that of C v at that temperature and plotted them C v versus temperature.

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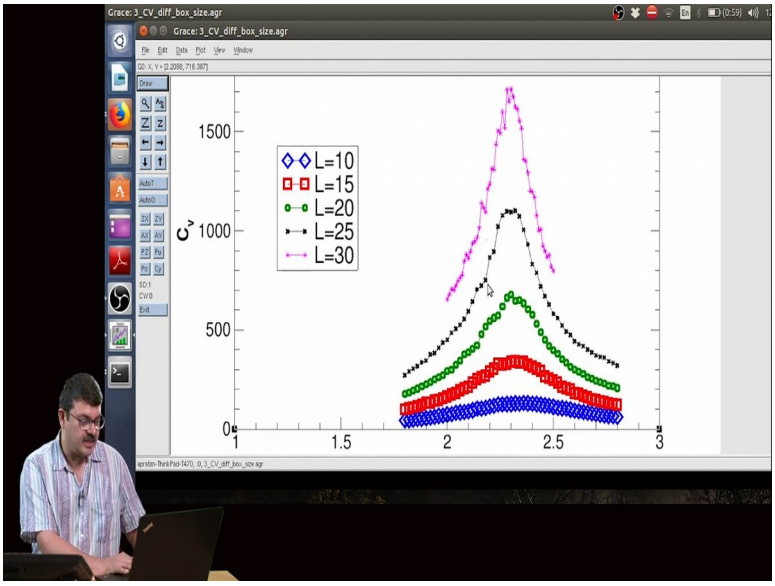

What do we see? We see that. As we increase the box size the peak sharpens, right. So, a smaller system has less fluctuations, a larger system can allow for larger fluctuations to happen, right.

Remember delta E by E goes as 1 by root N; but delta E or delta M the fluctuation magnetization goes as root N, you should plot that and check whether that is happens or not. So, the peak becomes sharper. So, the other thing that you can notice is the position of the peaks seems to move slightly to the left, as you increase box size, right. So, here there is a peak, it is not exactly clear. So, here there are large fluctuations and you can not exactly identify the peak; whereas, for smaller systems you have a relatively broad peak; but the position of the peak definitely shifts a bit to the left where wherever it be.

So, this might be better than M by plotting M or E versus N versus temperature, where it was getting very difficult to identify the transition here at least there is a distinct peak. But the position of the peak seems to change. So, this could be the transition temperature, but which transition temperature to choose; moreover we realize that for smaller systems averaging over 100000 iterations seems to be good enough.

But clearly for L equal to 30 which is this data, the data becomes noisy, there is not a smooth curve as one should expect right; it is not a smooth curve, even here you would see that there is a very broad peak, there are small fluctuations. So, what I have already done in the past noticing this is that, I ran for L equal to 30 instead of averaging getting the average value of C v by averaging over 10 to the power 5 iterations; I averaged over 5 into 10 to the power 5 iterations 500000 iterations at each temperature. And I also have that data here, which is shown in this maroon circles, filled circles and here you see a smooth data, right; a smooth curve you can clearly identify the peak right, you do not have any problems identifying the peak .

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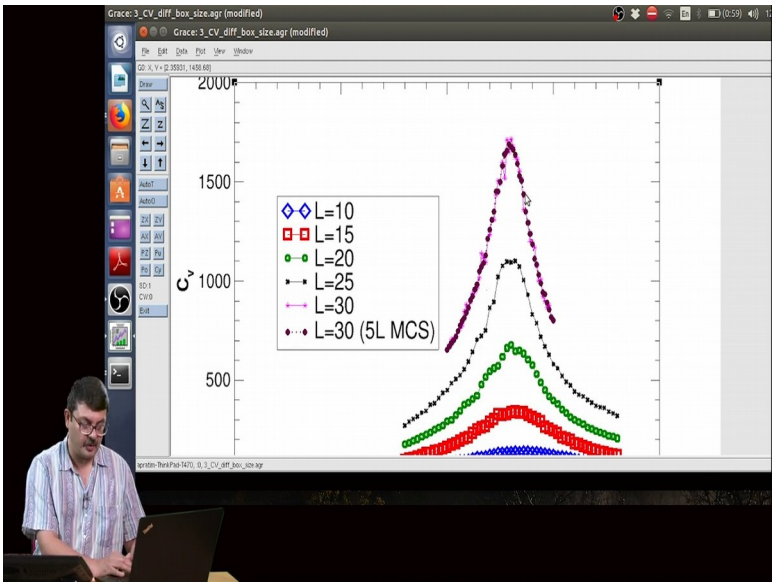

For smaller lattice sizes, 10 to the power 5 iterations was enough to calculate good values of the average of C v. But for larger systems you need to average better, because the fluctuations are more we need to average over larger number of iteration.

There is one more point; so such fluctuations in the value of C v you did not see that for the value of energy and magnetization right; and that part actually we have not even compared E and M for different box sizes. But let me tell you that the fluctuations in C v which is the basically the second moment in calculation of E is like fluctuation in E; you need larger number of iterations to average over compared to the number of iterations you need to calculate average values of E or M. Let us have a look at chi.

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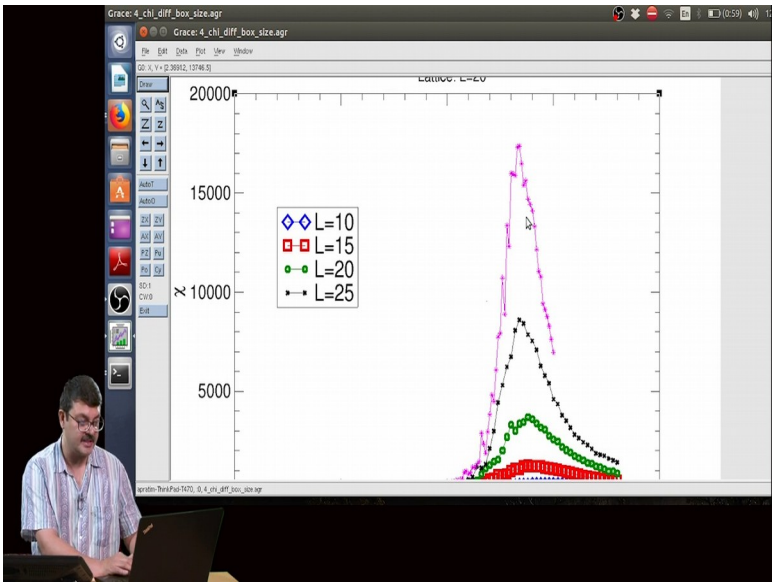

So, here again you see I have plotted chi versus temperature for different box sizes. And you see that there are, you see a clear peak the peak the sharpness of the peak increases with different box sizes, this is data for L equal to 30. And again you see that if you average over just 100000 iteration this is rather scraggy; that is not a smooth or good quality data are not good averaging.

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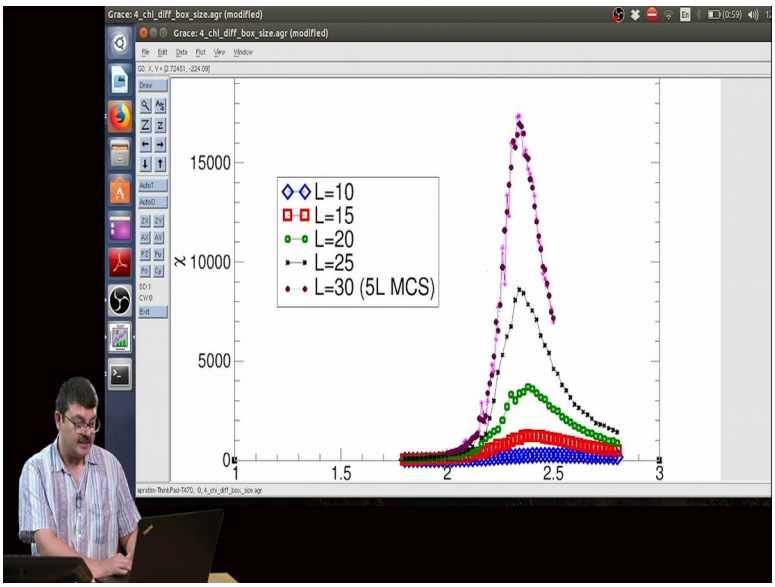

On the other hand if you averaged over 500000 iterations 5 into 10 to the power 5 iterations; then you get a relatively much smoother curve and you can easily identify the

position of the peak. But again you see that the position of the peak changes from this point, approximately if you look at, if you magnify this data here; you will see that the peak is somewhere around this point it has moved here. And then as you go up the position of the peak keeps on moving to the left.

In this case you are you face the problem, that which temperature shall you use to identify their transition, because if the transition temperature itself seems to depend upon the box size. So, as I shall introduce a bit later, one needs to calculate the so called Binders Cumulant, to identify the transition; and that is the actual transition temperature using Binders Cumulant we can find it out which we can compare with our experiment.

But here we are again seeing finite size lattice artifacts, right; as you change the box size the nature of or the position of the peak changes, which gives us, which makes us face the problem that how do we find out the correct transition temperature of the Ising model from the simulations.