Computational Physics
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Lecture – 24
Monte Carlo Simulation Analysis: Thermodynamic Quantities Part 02

But, before we discussed the Binder cumulant, I want to discuss some other stuff as well .

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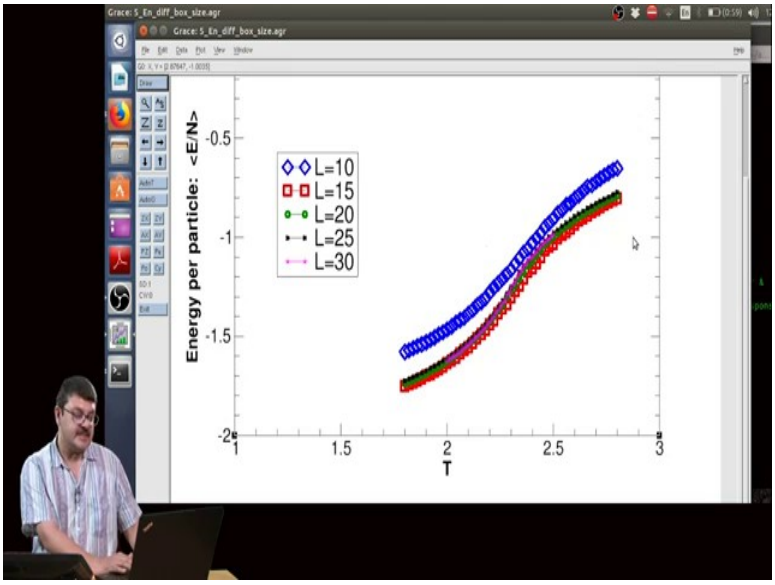

So, here what I have done is plotted the energy versus particle versus temperature for different box sizes and here we see and it is all over 1 lakh iterations only. So, at each temperature the average is averaging is over only 1 lakh iteration. This is L equal to 10 and this basically the magenta colored data, this is data for L equal to 30. And here we see that all the data is relatively smooth right. For CV if you remember for L equal to 30, when we averaged over 10 to the power 5 iterations we got scraggy data. The same for chi, but for energy or for M, you will get relatively smooth data right energy changes from around 0.5 to 1.5. This is all data for cooling curves.

So, I have started at a high temperature around 3 whether random initial condition allowed it to relax to equilibrium and then I am slowly changing temperature in decreasing the temperature. So, all the data that I have shown till now is for cooling

curves and here we see that even for L equal to 30 averages over 1 lakh iteration gives very good and smooth quality data. However, we did not see that for when we plotted the chi or when we plotted the CV and that is because we were looking at the fluctuations higher moments of the energy. So, CV and chi are higher moments of E and M basically standard deviation of E and M at every temperature, for that you need more averaging especially at larger box sizes right.

So, one has to be aware of these aspects. We could not just simply run and give or throw any data at you. You have to check whether they are good averaging, whether getting good quality data, even the data, that the quantity that you calculate does it capture the feature that you want to capture or understand from your simulations. In this case the magnet the ferromagnetic to paramagnetic transition so, basically in this graph I wanted to show you that E is relatively smooth it very smoothly with temperature over 1 lakh iterations. If you average over 1 lakh iteration so, that is enough but, not if you have higher moments, all right.

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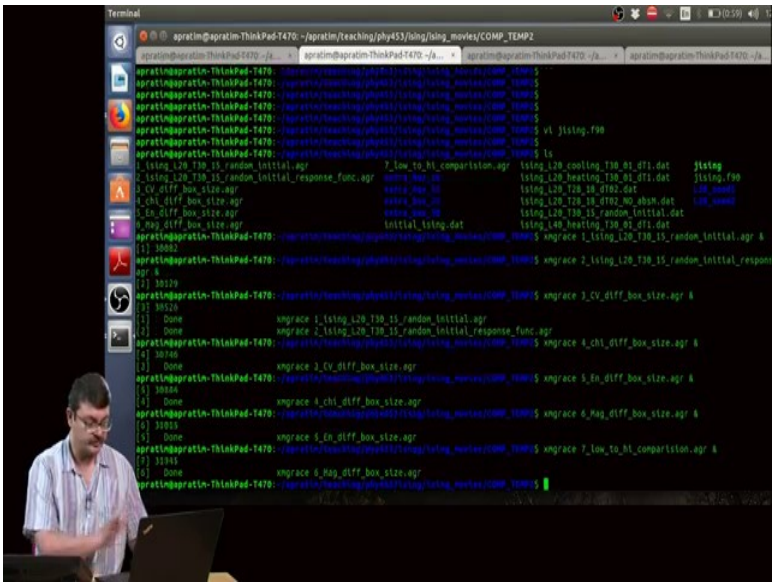

Now, to look at the next thing we explore is.

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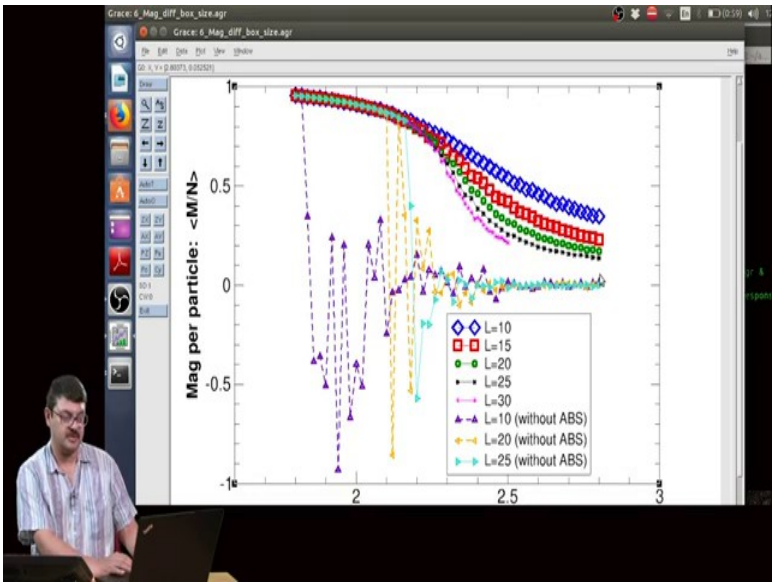

So, I have plotted magnetization versus temperature for different box sizes, where I have used this data L equal to 10, 15, 20, 25 and 30. I have used the absolute value of the magnetization while calculating average M I have used the magnetization at each micro-state. Whereas, this is data where I have not used the absolute value, I have basically averaged over M sometimes it is positive and negative.

And this is the difference in the quality of data that you get. For smaller lattices you have averaged it, but at higher temperature at temperature above 2.5 you should be getting 0, but you do get a finite value of the magnetization. Moreover, as you increase the size of the lattice this approaches closer and closer to 0 and the reason it reaches approaches closer and closer to 0 is basically as you have a larger lattice you have a larger number of spins which might be pointing up and down with equal probability.

So, when you average over a larger lattice the averaging is better it will be closer to 0. You will have an equal number of spins which might be pointing up and down which would correspond to a 0 magnetization state; whereas, for a smaller lattice size the fluctuation from the average the fluctuation from 0 will be more. So, that is why you are getting higher values here and lower values here. If you get go to bigger and bigger lattice sizes this is going to approach more and more 0.

However, if you calculate without M if we calculate M without taking the absolute value the ABS you are getting very accurate values of 0 here as it should as it as expected. But,

now near the transition temperature there are large fluctuations which you also saw it in the previous class, when we plotted magnetization versus MCS at a temperature of 2.15 you saw especially for small lattices and even for bigger lattices that M was rapidly changing from a positive value to a negative value from a negative value to a positive value.

And so, that aspect basically is shown and we can see that again here. So, this is basically very close to the transition temperature and you have the so called critical fluctuations as these temperatures. You have huge fluctuations basically the correlation length goes to infinity. We have not discussed correlation length I do not know whether you have had a stat physics class where it has been discussed we will discuss this briefly towards the end. But, here you have the so called critical fluctuations.

The entire system is going from positive to negative, negative to positive and hence sometimes the average is negative sometimes the average is positive. This is for L equal to 20 right and from such a data it is impossible to identify the critical temperature; whereas, if you take an absolute value at least you see this smoothly going from a value close to 0 to a value close to 1, corresponding term of a transition from the paramagnetic state to the ordered ferromagnetic state right.

And, furthermore you see that the larger the lattice size L equal to 25, here you have 0 with taking without ABS you see that there are some large fluctuations here, but around even above 2.1, it smoothly goes to suppose a positive state and it stays there right. Notice, that I have significantly increased the number of points here. So, the density of points between dt of 0.1 is around 4 here right because I want to the data to be smooth, I want a good quality data.

So, here I have chosen increasingly smaller values basically what how discrete, how small the value of dt is depends upon how accurately you want to calculate the transition. Of course, again you might have noticed that while initially the first data the dt was around 0.1, I went on decreasing the value of dt till I got the data of the accuracy and of the quality that I wanted. Simultaneously, I kept on also increasing the number of iterations over which I average.

But, the point is for a smaller box size you see that this transition is smeared over a larger temperature range. It keeps on fluctuating here and only here does it seem to settle down.

This is L equal to 10 whereas, for L equal to 20 it fluctuates widely near the critical temperature. This is the critical so called critical fluctuations and it settle downs here and after this it basically continuously decreasing to a value close to 1. So, most of the spins are pointing up here basically in the system. And for L equal to 25 this point is even sharper it reaches the smooth value here right.

So, this is the take home message, that it is better to use absolute value of M; the other solution is of course, to give a small biasing field in the beam B field so that one of the symmetry broken states is preferably chosen, then you increase the lattice size. The more you increase the lattice size you can take the thermodynamic average and then take B tends to 0. So, that is how it is calculated in theory ok. So, the last figure I wanted to show is a comparison of heating and cooling curves.

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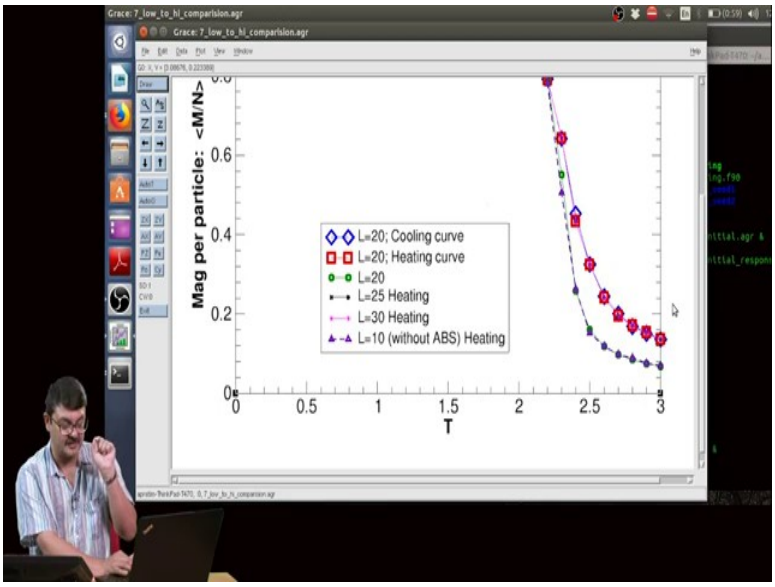

And the data is here. So, the first L equal to 20 was the cooling curve for L equal to 20. Basically, I started here and cooled it when down in temperature. The temperature range is 0.1 to 3. So, here I am looking at the entire curve. I have decreased the value of dt because I am basically comparing data not here the objective of this curve is basically not to necessarily to identify the critical temperature which I will be better of if I use CV or chi to identify the critical temperature right. But, here the point is to compare how the curves look.

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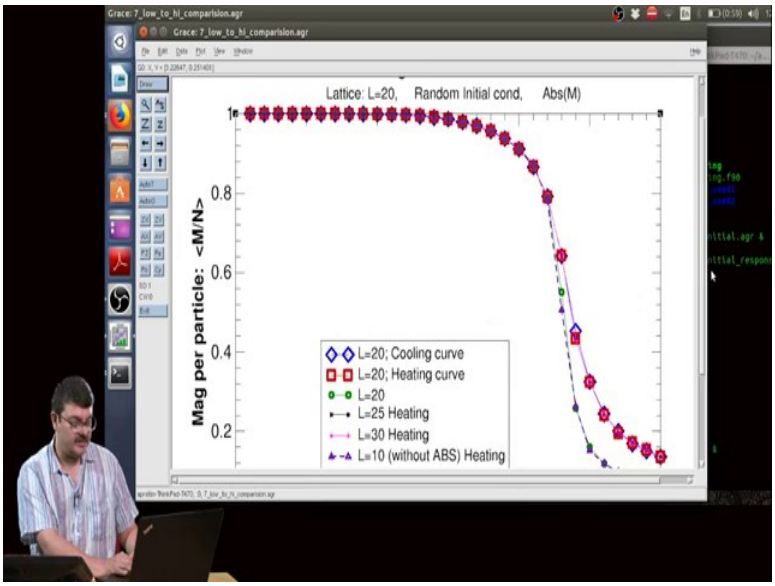

And, you see there is not much hysteresis. There is some size dependence here. Basically, when I take the absolute value it is coming like this. So, just how a stare, you will see that here they are basically in the most of the time they are falling on top of each other. This is the cooling curve, this is heating curves with different random number with different random number sequence and you see that you get the statistically similar data.

However, let me tell you sometimes in a heating curve when you start at a low temperature from random initial conditions once in a while it is possible that at low temperatures where you have long relaxation times, the system does not equilibrate does not reach equilibrium because thermal fluctuations are so slow the exploration of microstates different microstates also becomes very slow.

And one sometimes one gets weird values of weirdly low values of magnetization at low temperature. On increasing the temperature slightly the system is able to basically lower the relaxation time, so that the system is able to reach equilibrium faster and then it gets to some such value and then after that it basically follows this curve. I try to generate a random number sequence, so that I can show you when the system gets stuck and you do have non values of magnetization and not close to 1, some here values it fluctuates here and then as you increase the temperature it reaches a value close to 1 as it should and at higher temperatures of course, it goes to 0 as it should.

At low temperatures if you want to look up the thermodynamic quantities we want to calculate thermodynamic quantity especially at very low temperatures, when it is difficult to access different different micro-states one should use more advanced simulation techniques which will be out of the scope of this course. But, you can look up if you need it you can look up any proper Monte Carlo book it will be discussed in detail.