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**Lecture - 17**
**Monte Carlo Simulation**
**Introduction**
**Part 02**

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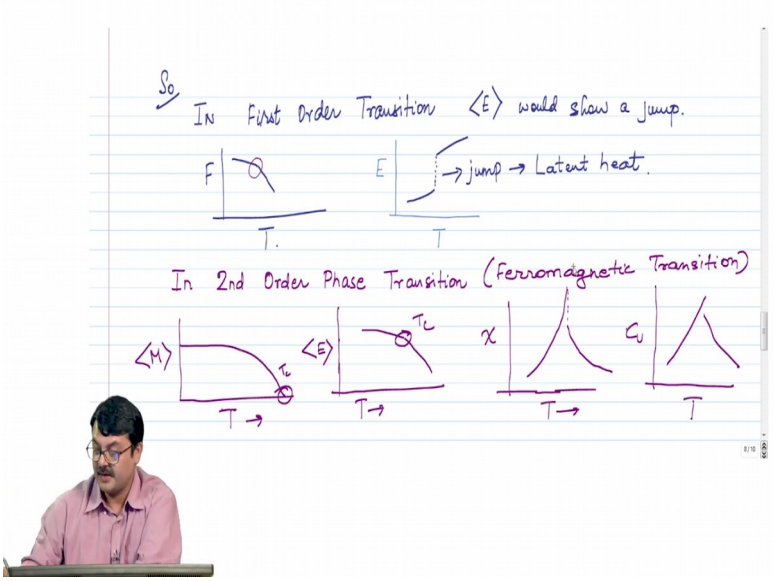


So, I shall explain the behavior of the free energies and bit more in detail, if you had a first order phase transition as I said average energy would show a jump. So, the free energy if you like as we increase the temperature for the first order phase transition case, it would be changing with respect to temperature. But, at the critical point, at the point of transition basically the slope would change. As a consequence the average energy of the system which is a measure of the slope of the free energy at every point in space it would show a jump right.

So, it shows a jump, it would be associated with the latent heat whereas, in a second order phase transition such as the ferromagnetic phase transition the magnetization which is the order parameter also in this case gradually changes and goes to 0, there is no jump. The energy would also not show any jump, it would change continuously. Of course the slope of this energy with respect to temperature would change, as a consequence in the second order;

in the second order derivatives of the free energy or del M del beta which is high or del E del T which is C v the specific heat capacity; they would show a jump and they would also show a singularity.

With this background of phase transitions you at least need this background of phase transitions and statistical physics because, when we model the so called Ising model to understand; basically the ferromagnetic to paramagnetic transition. I will be using this background language which we I just discussed to understand the system more.

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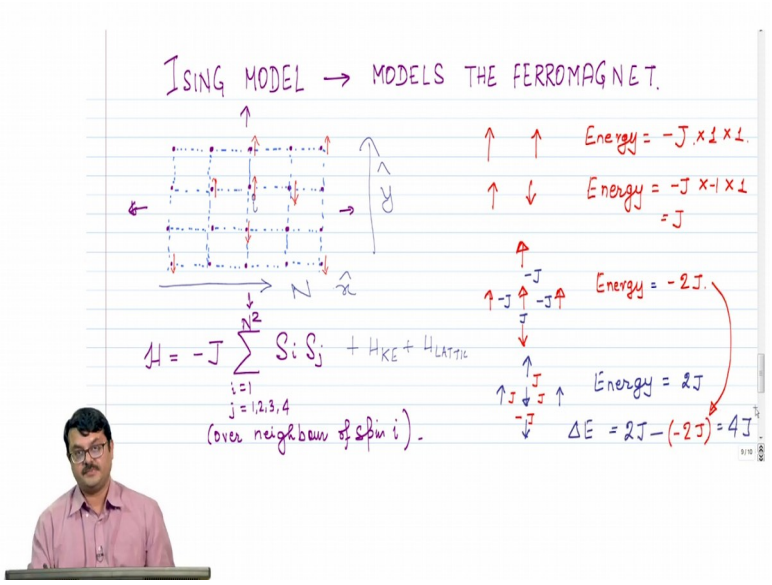


So, now let us focus on actually the Ising model and how and why Ising model models the so called ferromagnet at a finite temperature. Now, suppose you have a ferromagnet and suppose the ferromagnet has atoms basically sitting in a square lattice. So, basically these are the positions of atoms and there is already a background lattice, it is a square 2D lattice, one can also have a 3D lattice. And, basically at each point so, this is where the various atoms are sitting, each atom has a magnetic moment. So, this magnetic moment is essentially proportional to the spin of the system.

So, while I actually talk about the magnetic moment while, I actually mean the magnetic moment I shall be discussing or using the language that at each point in space there is an atom. And, you have essentially a spin which is pointing up or down. Magnetic moment and spin are of course, related by the Bohr magneton. Now, this is the so called Ising Hamiltonian and this describes only the ferromagnetic interaction between neighboring spins. So, basically

if this is a spin, these are the 4 neighboring spins of this one right. And, what the Ising model says that each spin can either point in the up direction or the down direction.

So, it has only 2 states plus 1 or minus 1 and furthermore the interaction between any spin with its neighboring spins is given by minus J, minus J is some coupling constant; we shall discuss this later. And, some constant basically for the purpose, for the present purpose just take it as some constant which sets the energy scale of the problem. The strength of interaction between 2 neighboring spins that is what is minus J and the interaction between 2 spins is given by S i into S j. So, the values that S i can take are plus 1 and minus 1 and the values that S j can take is plus 1 and minus 1 and basically you are summing over all the spins in the system. So, if there are N spins in the x direction say and there are N spins in the y direction say.

So, the total number of spins will be N square, where N is large taking the thermodynamic limit. And, you are essentially summing over all the spins i goes from 1 to N and j goes from 1, 2, 3, 4 all the neighbors of each spin i. The total interaction energy of the system is given by minus J summation i equal to 1 to N square S i S j j goes over 1, 2, 3, 4 which is the neighboring spins. Now, if you had a 3D lattice then each spin would have 6 neighboring spins not only this, this, this and this, but there would be 2 more spins in the z direction pointing along the plane of this board, you would have 6 spins and then the summation would be over 1, 2, 3, 4.

So over all the neighbors of spin i that is the message. So, this is the so called Ising model, the ferromagnetic Hamiltonian of course, the actual energy of the system would also consist of the kinetic energy and other interactions which keep the lattice in place. But, here we are focusing only on the relevant degrees of freedom to understand the ferromagnetic to paramagnetic transition. Hence, we are ignoring the other terms which are of course there, say the kinetic energy or the interaction between atoms which keeps the lattice in space or phonons and so on so forth. But, here we are basically focusing only on the part the interaction between spins which gives rise to the net magnetic moment of the system.

So, other degrees of freedom we are we will not be considering in our simulations. Now, let us focus with this background let us focus on how one would calculate the energy. Now, if one had 2 neighboring spins pointing in the same direction, the energy would be minus J S i into S j both are plus 1. So, the energy would be basically minus J, if you had 2 spins which

are pointing opposite to each other then the energy would be minus J into minus 1 one of these spins has minus 1 spin and the other is plus 1 so, it is the energy is J. So, what is the message? 2 spins 2 neighboring spins pointing in opposite directions have a positive have a energy of J whereas, 2 spins pointing in the same direction have energy minus J.

So, at 0 temperature where there are no thermal fluctuations the system will evolve or the spins would all like to point in the same direction so that its energy is minimized. Actually in a thermodynamic system what is minimized is the free energy and not the energy, but at T equal to 0 what is left of the free energy is basically only the internal energy u. And, that will be and that is the quantity which will be minimized of course, at a higher temperature the free energy will have both u minus T s. So, there will be a competition between u and T s and that can lead rise to phase transitions as we shall see further in the lecture. Now, suppose one has a spin as I showed you here and it is surrounded by 4 spins.

So, this spin central spin has 3 spins which are pointing in the same direction as the middle spin and one of the spins, one of its neighboring spins is pointing in the opposite direction. Then the energy of this configuration would be minus J minus  minus J plus J which is minus 2 J, now suppose the central spin was flipped. So, here you see that the central spin is pointing in the bottom direction, the configuration of the other neighboring spins remains the same and you can easily see that the energy of such a configuration is J J J minus J which is energy of 2 J. So, basically if this spin flipped from plus 1 to minus 1 the net change in energy is 2 J minus 2 J which is 4 J.

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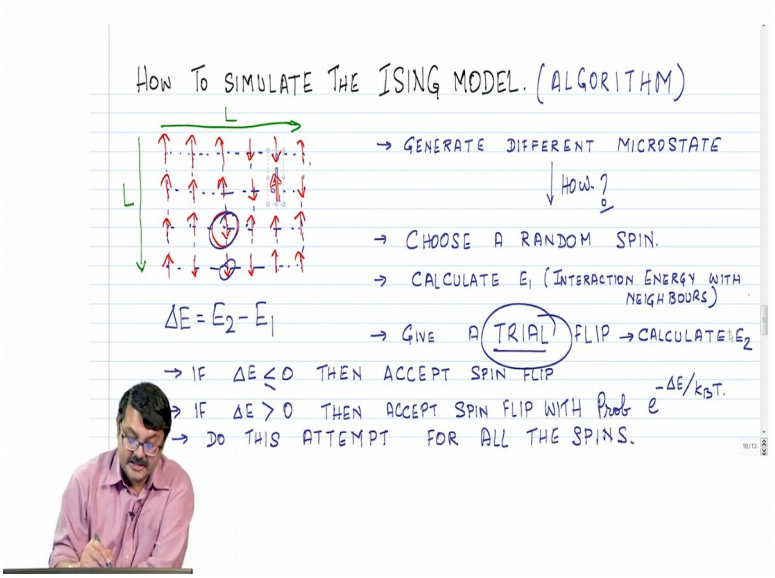


So, now that we have learnt a bit about the Ising model, the question is how do we go about simulating the Ising model. So, what is the general picture? Algorithm. Now suppose that you have basically n spins sitting in a lattice of size L by L. So, you have all these spins sitting here, here some are up, some are down and to do the statistical mechanics with the Ising model one basically has to generate different microstates. So, how do we go about generating different microstates? So, this is suppose some initial configuration where some spins are up and some spins are down and the way we go about generating different microstates is that we choose a random spin.

So, just suppose that you choose a random spin suppose this one and it is surrounded by its nearest neighbors which is this spin, this spin, this spin and this spin. So now, you can calculate the energy of interaction of this central spin with its 4 neighbors. And, next what we do is basically give it a trial spin flip which means, if the spin is pointing down means its value is minus 1 say then you say that I give it a spin flip. So, that it is now pointing up, this will lead basically to a different energy of interaction with its neighbors and suppose that value of the energy is E 2. So, when it was pointing down, suppose that the energy was E 1 and now that it has been given a trial spin flip the energy is E 2. So, it is a different energy because, it is pointing in different directions right.

So, the Monte Carlo simulation technique says and I will tell you why and I will slowly explain and maybe the later classes. But, the algorithm goes as if this energy change has been

negative or 0 which means the on flipping the spin the energy has actually decreased, then we accept the spin flip with probability 1. On the other hand due to the spin flip, if the change in energy has been E 2 has been delta E which is greater than 0. What is delta E? Delta E is E 2 minus E 1, if this delta E is greater than 0 then except the spin flip with probability e to the power delta E by K B T. This delta E by K B T it might remind you of the so called Boltzmann factor of statistical mechanics right.

So, whether a spin flip attempt is successful or not, that depends really on the change in energy due to the spin flip, if less than 0 or equal to 0 accept it, if it is greater than 0 then you accept it with only a certain probability. So, that is how you basically spin or rather you flip a single spin. Now, we have to do this for all the spins at the end of n trials you basically attempt a spin flip with all the spins. Now, at the end of n trials when all spins have been attempted to be flipped some of them would flip and some of them will not, depending upon the energy; change in energy when you flip a spin you essentially get a different microstate. Because, then some of the spins would be pointing, say in the opposite direction; suppose this, this, this, this and you have essentially a different microstate.

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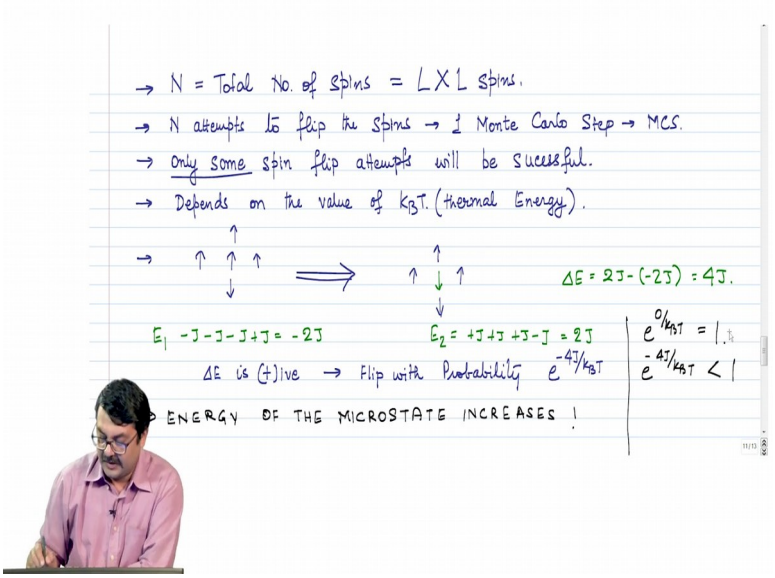


So, suppose that N is the total number of spins. So, N is essentially L cross L, you just remind you what is L; L is the number of spins suppose in the x direction and in the y direction. So, it is a square lattice, you have spin sitting on the lattice and you have L spins in this, L spins in this. So, basically you have N the total number of spins is L cross L. So, if you make N

attempts to flip this spins that is called 1 Monte Carlo steps. So, what is 1 Monte Carlo step? You have N spins in the lattice, you have made N attempts to flip this spin; some of those attempts are successful, some are not right.

And, basically how many spin flip attempts will be successful depends essentially on the value of the thermal energy which is basically given by K B T. And, why is that so? Let us whatever I told in general principle let it let me break it down into slightly detailed algorithm right, let us focus on the spin flip of a particular spin say this one. So now, this is surrounded by this spin, this spin, this spin and this spin. So, the energy of interaction of this particular spin with its neighbors is basically minus J due to this, then the next one is again minus J, next one is again minus J and the last one is plus J because they are pointing in the opposite direction right and the total energy of interaction of this spin with its neighbors is basically minus 2 J.

Of course there are also other spins in the lattice also surrounding it which I have not drawn, but they are there. And, when we consider the spin flips of the other spins then we have will focus on one other particular spin, suppose sitting somewhere here and then basically look at its neighbors. Now, if the spin is flipped then basically it is pointing in the opposite direction and the energy of this configuration will be E 2 which now will be plus J because, now this and this are pointing in the opposite direction right; plus J plus J plus J and minus J. So, the energy of this new configuration is 2 J, the change in energy is of course, 4 J now you can calculate 2 J minus minus 2 J. And, the point is so, on this trial spin flip the energy is not decreasing actually, but increasing right from minus 2 J to plus 2 J.

So, if the energy change is positive; what I told you is basically you flip the spin with probability e to the power minus delta E, delta E being 4 J by K B T right. So, that is the probability of acceptance, just to tell you that e to the power is 0 by K B T is equal to 1. So, e to the power 0 is 1 right and e to the power minus 4 J by K B T where J is positive that will be some number less than 1. So, you can talk about probability, if the energy change was negative energy had decreased then basically this delta E would be negative, e to the power minus minus delta E would be a positive which is any way greater than 1. So, that is how you flip a spin a particular spin; now we have to do this for all this spins one by one to have 1 Monte Carlo step.

Now, at the end of this due to the end of due to the change of the state of 1 spin, I want you to realize that the energy of the microstate has increased right; previously this particular configuration had energy minus 2 J, now it has energy plus 2 J. So, if you look at the entire lattice other spins being exactly the same as before, due to this particular spin flip the energy of the microstate has increased. Where is this energy coming from?

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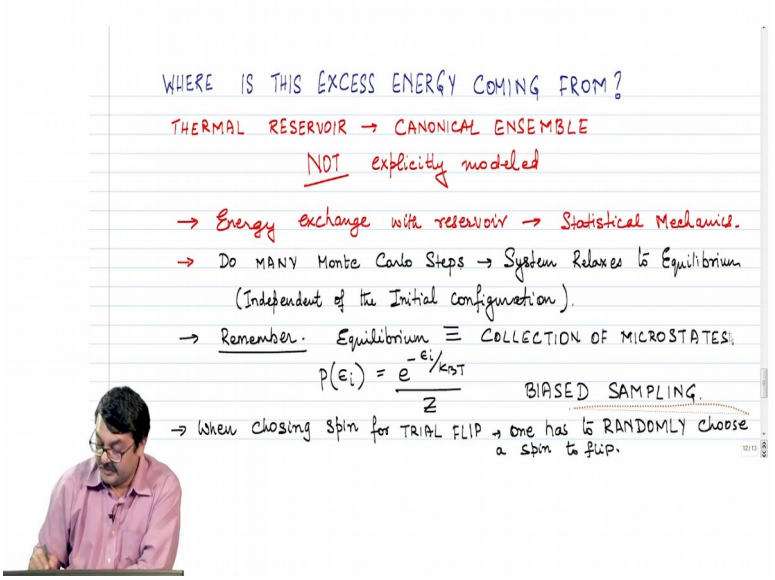


So, the question is where is this excess energy coming from? The point is that there is a thermal reservoir. So, we are actually in the Ising model when we try to do this in a spin flips and energy changes there is a thermal reservoir as in a canonical ensemble. So, we are actually working or looking at magnetism in the canonical ensemble, the thermal reservoir is not explicitly modeled. So, it is there somewhere, but we are not modeling it because our focus is basically what these spins are doing, basically what are these spins are doing. But, there is a thermal reservoir and this system is basically interacting with that thermal reservoir which is not explicitly modeled.

So, when there is a spin flip there is an increase in energy, basically the system is taking energy from that reservoir and when there is a spin flip such that the energy of the entire system decreases. So, that you have a microstate with a lower value of the energy, basically the system has given some energy to the reservoir. So, you understand that you have an energy exchange with a reservoir and basically we are talking statistical physics and statistical mechanics right. So, when you have many Monte Carlo steps; so, we do many

Monte Carlo steps which means we have a lattice, we flip, we give a trial, spin flip to one of the spins then we give N trials spin flip which is 1 Monte Carlo step.

Now, we do this over and over again which means we give N trial spin flips over and over again to all the spins on an average, then basically the system relaxes to equilibrium. What is equilibrium? Basically, equilibrium is a collection of many microstates right and independent of from what initial condition you have started out with, when you do many Monte Carlo steps you will reach equilibrium this collection of different microstates, there will be a certain number of spins on an average pointing up, a certain number of spins pointing down. The system is continuously accessing different microstates because, different at the next instant after 1 Monte Carlo step a different number of spins are pointing up and down.

But, it will basically fluctuate about an average that is what we do in statistical mechanics; calculate the average quantities thermodynamic average quantities in equilibrium. And, it is equilibrium if basically the probability of accessing different microstates with different energy E i energy E i is so, different microstates are accessed with the probability e to the power minus E i by K B T divided by z, where z is the partition function which is basically the probability of accessing different microstates in a canonical ensemble. Now, here I want to point out that while we are changing, we are flipping spins we are changing from one microstate to the other, all microstates are not accessed with equal probability.

You know if there is an energy change which is negative, we are always accessing the; we are always accepting the spin flip. If the energy increases on a trial spin flip, we are axis we are accepting the move with a probability e to the power minus delta E by K B T. So, all the microstates are not being accessed with equal probability right and that is what; that is what basically you have in a canonical ensemble and we are basically a sampling, we are doing a bias sampling of states. You could have also done that basically you access all microstates with equal probability and then calculate the energy. And so, energy is the average energy would be essentially E i energy of the microstate into probability of accessing the microstate right.

So, that is also possible, but here we are doing a bias sampling. So, that we are accessing microstates with the probability e to the power minus E i by b K B T. So now, basically for each microstate, if you calculate the energy and calculate the average energy. Since, these microstates are themselves are being accessed in a biased manner as e to as per basically the

canonical ensemble; we can just calculate average over the different energies of each microstate. And, we will get the average energy of the system right so now, I am connecting with statistical physics. A point to remember is that when choosing a spin for a trial flip one has to randomly choose the spin to flip. So, you do not go from one end of the lattice to the other one by one because, that essentially introduces some artifacts in the system.

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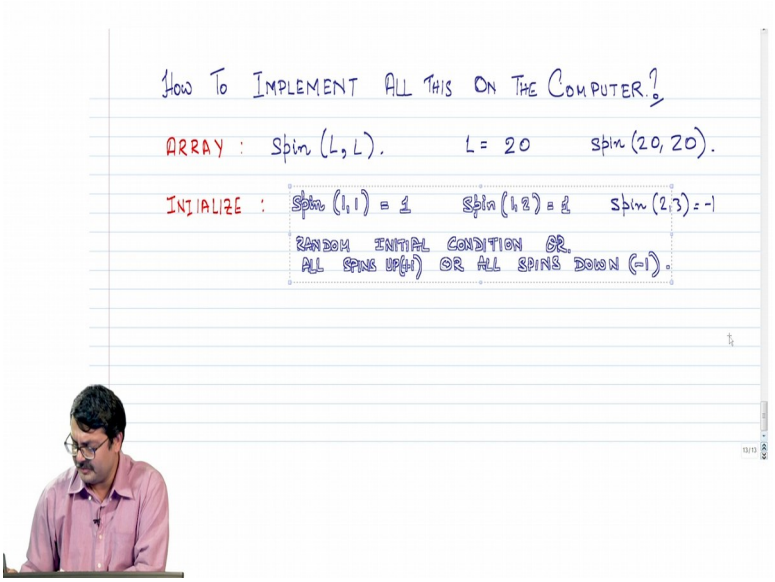


Finally, I would like to end the class by we have discussed a lot about Ising model, phase transitions, then how to implement it, but all this how do we implement it on the computer; we will be talking about it in detail in the next class, we will just give an idea about where we are heading. You know so, we said in 2 flips and 2 slides before that you basically have arranged spins on a lattice; some of them are pointing up, some of them are pointing down. So, there is a square lattice corresponding to that on the computer, what you are going to have is a square array right.

So, have an array spin L cross L, L was the length of that lattice in one direction x and y direction. So, L cross L is n suppose L is 20 so, you will define an array spin 20 cross 20. Now, you can initialize the spin. So, how do you initialize the spin? You go to each element of this array say 1 1 and say ok. So, I assign 1 to it, 1 means spin pointing up and you say spin 1, 2 at the second point in the on the lattice, the spin is again pointing up and then you go to 1 3 and 1 4 and 1 5 and up till 1 20. So, basically you have assigned the spins in along 1 axis and then you go to spin 2 3 and suppose you give it minus 1 right. So, this way going to

each of the elements of the array, this array basically defines your lattice; you are assigning spins to each of your lattice points or if you like array points.

You could have a random initial condition which means all the spins at each point in the array have either plus 1 or minus 1 chosen randomly by using a random number generator. Remember we are doing Monte Carlo simulations so; random number generator will come up over and over again. Also, while choosing probabilities and when flipping a spin or you could basically say I am going to set all spins up plus 1. So, all the elements in that array spin L L have plus 1 or all the spins are minus 1, spins are pointing down. It really does not matter because, you are going to do Monte Carlo simulations, you are going to do MCS and after MCS the system is going to reach equilibrium at that temperature.

And, basically what is going to happen is the equilibrium, the set of microstates which constitute the equilibrium thermodynamic state are independent of the initial condition right; it depends only on the temperature. Why on the temperature? Just let me remind you now, suppose you had this configuration and it was going from this configuration to this configuration right. And, you know that the energy change is 2 J, but if you have a different value of K B T then basically this probability of flip changes because, 4 J remains constant if it goes from here to here. But, the value of K B T will be different so, this factor this the value of this factor independent will be different values. So, the probability of acceptance will be different.

Of course, there could be also different configuration, not only this configuration then the value of delta E will be different. But, if it is at a different temperature anyway that prefactor is going to be different, the probability of flip is going to be different. So, it is going to access different set of microstates or the same set of microstates, but with different probability function right. So, in the next class we will go down a bit more in gory details, look at the algorithm in more detail, how we are going to implement it, I am going to show you a simple code in 2D right and your job will be to implement the same thing in 3D. So, but let us wait till the next class.

Thank you.