# Computational Physics
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## Lecture – 25
## Monte Carlo Simulation Analysis: Thermodynamic Quantities Part 03

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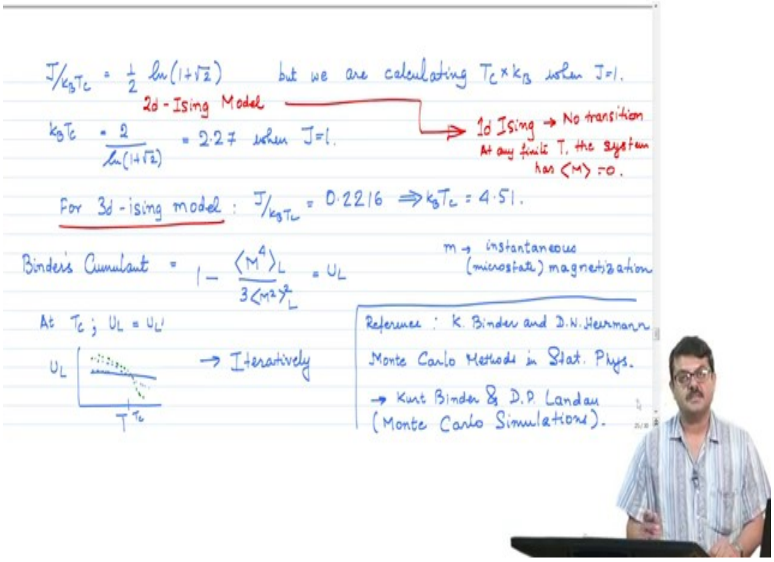

$J/k_BT_c = \frac{1}{2}\ln(1+\sqrt{2})$ but we are calculating $T_c \times k_B$ when $J=1$.

2d - Ising Model $\rightarrow$ 1d Ising → No transition
At any finite T, the system has $\langle M \rangle = 0$.

$k_BT_c = \frac{2}{\ln(1+\sqrt{2})} = 2.27$ when $J=1$.

For 3d - ising model : $J/k_BT_c = 0.2216 \Rightarrow k_BT_c = 4.51$.

Binder's Cumulant $= 1 - \frac{\langle M^4\rangle_L}{3\langle M^2\rangle_L^2} = U_L$

$m \rightarrow$ instantaneous (microstate) magnetization

At $T_c$ ; $U_L = U_{L'}$

→ Iteratively

Reference : K. Binder and D.W. Heermann
Monte Carlo Methods in Stat. Phys.
→ Kurt Binder & D.P. Landau
(Monte Carlo Simulations).

Coming back to the slides the value of the critical temperature for the 2D Ising model, it can be calculated exactly and the value of J by k B T k B T C is half ln of 1 plus root 2, but in our case we have set J equal to 1 and we are measuring temperature in units of J. So, in that case we putting J equal to 1 the value of k B T C will be exactly this factor and it is 2 by ln of 1 by root 2. And, when you put in the numbers the value comes out to be 2.27 when J equal to 1. And that is exactly what we saw right there the peak in the CV and the chi was in this range it was below 3, but above 2.2 definitely and of course, the peak was shifting.

The problem remains since the position of the peak were shifting continuously how do we calculate the value of T C right? For the 2D Ising model of course, it can be calculated exactly we are doing we are implementing the 2D Ising model on the computer because we can exactly check, but for the 3D Ising model as of date nobody can calculate the value of the critical temperature accurately. By the way just let me tell you that by computer simulations and also by analytical techniques which are approximate you are you can be accurate only up to a certain degree the value of the of J by k B T C for the 3D Ising model is known and it is value is 0.2216 right and if you set J equal to 1 if you measure temperature in units of J which is what we have been doing till now.

Then, the value of k B T C comes out to be 4.51 is basically one of one by this number right. Just for the sake of completeness I think I have said this before that, in the 1D Ising model. So, when all those spins are placed along a line so that each spin has just two neighbors, so, on the two sides and this was proposed by Ising sometime in the 1920s and Ising did not find any phase transition. What does it mean? It means that as soon as there is any finite value of temperature the tiniest T value going very close to 0 right as soon as there is a finite value of the temperature there is no order in the system, that is that the average magnetization goes to 0 all right.

So, there is no transition only at T equal to 0 do you find that all spins are either pointing up or down but, at any finite temperature and it can be calculated easily for the 1D case he found that the transition is 0. So, he gave up without the model is of no use and it took some quite a few years 20 – 25 years before Onsagar could calculate it exactly, could analyze the Ising model exactly in the 2D case, for the 2D Ising model and use the sum transfer matrix formalism which you should read up in your statistical mechanics book if you are interested in the topic.

And, there you found that yes at any finite temperature there is an ordered state, there is a large number of spins pointing in the same direction so, say the positive direction. And only when a temperature is raised above a certain critical temperature do you get disorder in the 1D at any small finite temperature you will getting disorder, in 2D we are getting disorder only when the temperature is raised above a certain value right and of course, different systems would have different values of J, I mean where or what you could do that if a system is has interacting spins which in the Ising case, you find out the T C and back calculate to the J that is also possible and for 3D of course, it is even higher value in terms of J .

The problem remains that for suppose the 2D or the 3D case and suppose you did not know the T C, then how would you figure out or how would you calculate the exact value of T C. Specially since there has been significant finite size affects the value of the T C they have the value of the peak in the CV and the chi were shifting to the left as you went higher and higher, box size is larger and larger box sizes.

The way you do it is by calculating the so called Binders Cumulant and where it comes from and so on so forth is out of the scope of this course. One needs some more statistical physics, some scaling theories and finite size scaling analysis to understand from where this Binders Cumulant comes from, here I shall simply tell you the method how to identify the exact critical point. So, what one has to do is calculate the Binders Cumulant which is 1 minus M to the power 4 expectation value by 3 M square expectation value at each micro scale state calculate the value of M, M square calculate the expectation value and then take a whole square and note that here I have written basically a subscript L here and a subscript L here.

So, for different box sizes for different lattice sizes you can calculate M 4 average, calculate M square average, square it, calculate this quantity entire quantity this is called U of L or the business cumulant. Now you can calculate this quantity for different box sizes different values of L. And, at T C the values of the Binder Cumulant is exactly the same independent of the box size.As I said before where and why this happens we are not discussing this that is outside the scope of the course, but what you could do is calculate U L versus the temperature for different box sizes near the critical point.

So, basically suppose this blue line and the green line and the dashed line they are for different box sizes, you are calculating U of L near the critical temperature and plotting it as a function of temperature in these different lines or box sizes and at the critical temperature all the lines will intersect. So, the point of intersection is essentially the critical temperature.

Now, let me tell you I mean you are supposed to do it for your homework. But, let me tell you that to calculate the critical temperature exactly one has to do it iteratively which means like you already know from the data that you have seen that basically the critical temperature lies between 2.2 and 2.3. So, take different values of dt small values of dt, change the temperature from 2.2 to 2.3. Calculate U of L plot it as a function of temperature for different box sizes and what you will see is, the different lines nearly seem to intersect at a point, but not exactly.

But, once you identify the player the approximate range of the temperature where it is approximately intersecting, now again run the simulations for even smaller values of temperature over a smaller temperature range nearer the critical temperature and if you do it iteratively you will come across a temperature you will come across a point value of T where all the lines intersect and that is your critical temperature and that is what it means by doing it iteratively. If you want to know more about it details the background theory and much better analysis has been discussed very well by none other than Kurt Binder on whom the Binder's Cumulant is named.

So, there is a book by Kurt Binder and Dieter, D. W Heermann;  and the book is called Monte Carlo methods in statistical physics want to know Monte Carlo methods in statistical physics in greater detail. There is also a book by Kurt Binder and D. P Landau and it is called Monte Carlo Simulations. This is a quite an advanced book, it really discusses all the advance techniques. If you are learning Monte Carlo simulations I would advise you to refer to this book; if you are already an expert and want to know advanced techniques then this is the method.

In this course the aim is not to make you an expert in Monte Carlo, but basically expose different types of computational methods to you, so that whether you do stat mech or you do space science or gravity or whatever be it, material science, you can develop the skill set to go into that research area, do the calculations, implement the code and test it out. So, our aim is not to have a great or detailed understanding of a Monte Carlo simulations or physics of phase transitions, this is just an exposure.

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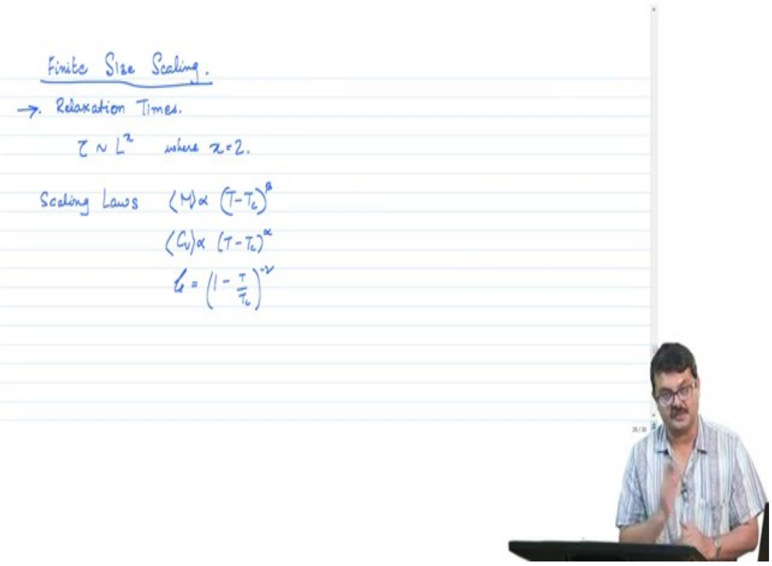

Finite Size Scaling.

→. Relaxation Times.

$\tau \sim L^{x}$ where $x = 2$.

Scaling Laws $\langle M \rangle \propto (T-T_c)^{\beta}$

$\langle C_v \rangle \propto (T-T_c)^{\alpha}$

$\xi = \left(1-\frac{T}{T_c}\right)^{-\nu}$

Just to let you know so, we will be stopping with within the next 10 minutes, but if you have wanted to know more there is the entire phenomena of finite size scaling, there is the scaling laws, this is critical phenomena. So, even in the Ising model as you go close to the critical temperature various quantities such as the magnetization, the CV, the correlation length they show certain scaling laws and that is within the realm of critical phenomena.

So, unless you know more about statistical physics and critical phenomena it would not be relevant to discuss those points in detail. But, the point I am trying to make is I just give you give you a brief exposure to Ising model simulations, just to have an idea how to model things on a lattice, find out its properties and implement boundary conditions and so on so forth.

Just to let you know in our current simulations the ones which I showed you I we were calculating we were collecting data to calculate thermodynamic averages – average e, average m every Monte Carlo step right every Monte Carlo step we were calculating it, that is for overkill, one should basically take thermodynamic averages over microstates which are not linked which are statistically independent of the previous microstate. In one Monte Carlo simulation it is not necessary that you will get independent microstate that is particularly true at lower temperatures.

And, here I want to mention that to do it properly to figure out whether you are getting independent microstates at the end of every Monte Carlo iteration, one Monte Carlo step one has to calculate the so called relaxation time and the relaxation time specially goes as L square L to the power x, where x equal to 2 for a 2-dimensional lattice and what one should ideally do is take this data after every a few MCS and it really depends whether the check and it is really important to check whether these microstates over which you are collecting data to calculate thermodynamic averages are statistically independent or not.

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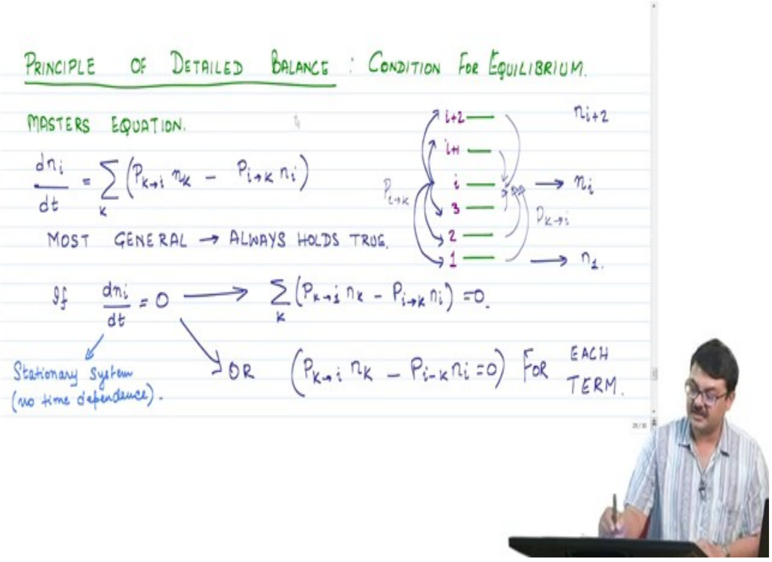

PRINCIPLE OF DETAILED BALANCE : CONDITION FOR EQUILIBRIUM.

MASTERS EQUATION.

$$\frac{dn_i}{dt} = \sum_k \left(P_{k\to i}\, n_k - P_{i\to k}\, n_i\right)$$

MOST GENERAL → ALWAYS HOLDS TRUE.

If $\frac{dn_i}{dt} = 0 \longrightarrow \sum_k \left(P_{k\to i}\, n_k - P_{i\to k}\, n_i\right) = 0.$

Stationary system (no time dependence).

OR $\left(P_{k\to i}\, n_k - P_{i\to k}\, n_i = 0\right)$ FOR EACH TERM.

So, we shall end this module with a last point which is basically discussing the principle of detailed balance. Till now, I have been when I have been discussing the algorithm, I have been basically telling you that you know to implement the metropolis algorithm an important sampling way what you should do is, flip give a trial flip to a spin selected randomly. If due to this flip the energy of the system locally over the spin and the system decreases accept the trial flip; however, if due to the trial flip the energy of the system increases then accept it with probability e to the power delta e by k B T.

Now, you have been asked to simply accept that, but where does this algorithm which I basically dictated to you come from? And that comes from the principle of detailed balance it comes from statistical physics. Now, what is the principle of detailed balance? So, for that we have to discuss the so called masters equation. Masters equation is an extremely general generic equation. Now, suppose that you have a set of states . So, 1, 2, 3, 4 so on so forth and in general called one of the states these are energy states to be i ok.

And, suppose that in each of these energy states there is a certain number of particles later we will change the language from particles to microstates, but for the simplicity just we will make that analogy later, but suppose there are some discrete energy states 1, 2, 3, 4 with energies e 1, e 2, e 3, e 4, e i, e i plus 1 and e i plus 2 and so on so forth and each has a population number of particles if you like n 1, n 2, n 3, n 4, n i and then higher state is n i plus 1 ok.

And, due to some background physics suppose the number of particles in each state in supposed state i which let us focus on that on the energy state i that can change. How can it change? Because particles will jump from i to suppose energy state 3 or 2 or 1 or i plus 2 and so on and so forth. And, so, basically from here particles are jumping to different energy states and similarly, from other energy states there are particles which are jumping into state i.

In that case one can write in the most general manner the so called master's equation which says dn i dt, the number of change in the population of state i as a function of time that depends upon P K i's; so, the probability of hopping from state K to state i from state K to state i and the population of state K. So, suppose K will be 1, 2, 3, 4, i plus 2, i plus 1 all states except i sum over K a K goes over all the states and this comes with a positive number because from different states particles are hopping into state i, so, transition from K to i population of n K right.

So, it will depend upon this transition probability multiplied by the population density of a state K minus so, from each from state i there is a certain transition probability for number of particles to go to state 3, 2, 1 and so on so forth in general from i to K the transition probability i to K into number of particles in state i and this comes with a minus sign because as particles hop the transition from state i to other states in other energy states, the population density of i decreases. Hence there is a negative sign here right.

And, this equation will always be true in general P K I could also be a function of time, but if it is not, if one has a so called stationary state in that that the population densities in each of these states are not changing as a function of time. So, dn i dt equal to 0 say so, that would be a stationary state and that can happen in two ways.

Now, let us focus on state i right and that can happen if the sum is 0 as a whole. Alternatively, if each of these terms in the bracket are 0 so, basically this quantity is 0 for each term individually right and then also you can have that dn i dt equal to 0 which is a stationary state.

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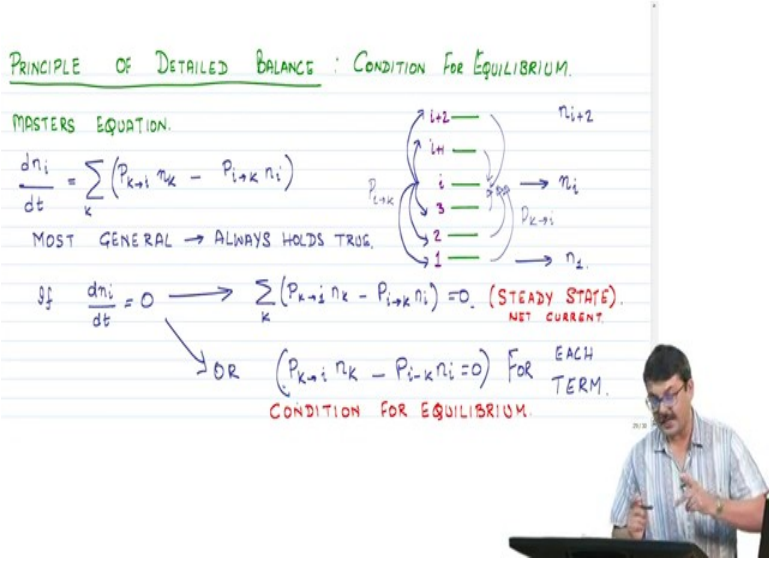

PRINCIPLE OF DETAILED BALANCE : CONDITION FOR EQUILIBRIUM.

MASTERS EQUATION.

$$\frac{dn_i}{dt} = \sum_K \left( P_{K \to i}\, n_K - P_{i \to K}\, n_i \right)$$

MOST GENERAL → ALWAYS HOLDS TRUE.

$$\text{If } \frac{dn_i}{dt} = 0 \longrightarrow \sum_K \left( P_{K \to i}\, n_K - P_{i \to K}\, n_i \right) = 0. \quad \text{(STEADY STATE).}$$

NET CURRENT.

$$\text{OR} \quad \left( P_{K \to i}\, n_K - P_{i-K}\, n_i = 0 \right) \text{ FOR EACH TERM.}$$

CONDITION FOR EQUILIBRIUM.

Now, if there was a current from any pair of state, so that only the sum of the sum which was on the right hand side of the equation is 0 the sum is 0, then also you can have dn i d dt then you what you have is a steady state. Basically, there is a net flux of particles from one state to the other i to i plus 1 or negative current if there is from particles going from 2 to i and so on so forth and that is when you have a steady state.

On the other hand, if each term in the bracket this term is equal to 0, that is a condition for equilibrium. So, individually for any pair of states i and K, if this condition holds, that is a condition for equilibrium.

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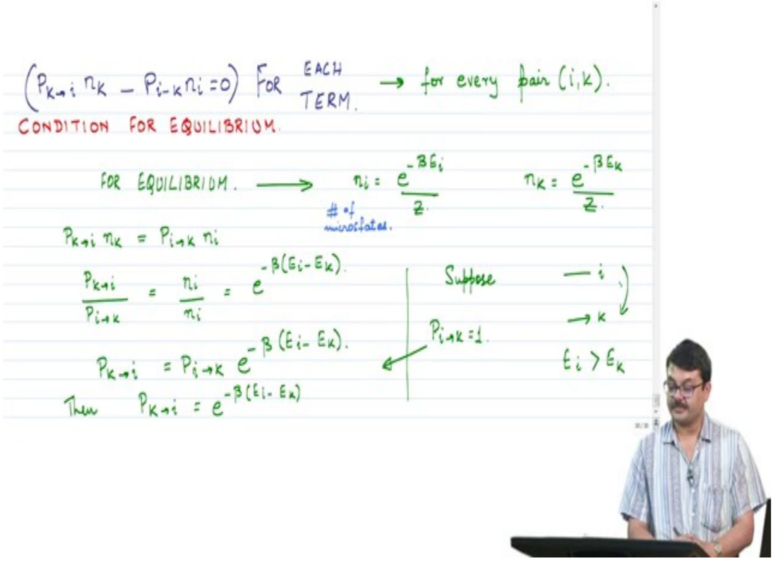

$(P_{k\to i} n_k - P_{i\to k} n_i = 0)$ FOR EACH TERM. → for every pair (i,k).

CONDITION FOR EQUILIBRIUM.

FOR EQUILIBRIUM. ⟶ $n_i = \frac{e^{-\beta E_i}}{Z}$ # of microstates. $n_k = \frac{e^{-\beta E_k}}{Z}$

$P_{k\to i} n_k = P_{i\to k} n_i$

$\frac{P_{k\to i}}{P_{i\to k}} = \frac{n_i}{n_i} = e^{-\beta(E_i - E_k)}$

$P_{k\to i} = P_{i\to k} e^{-\beta(E_i - E_k)}$

Then $P_{k\to i} = e^{-\beta(E_i - E_k)}$

Suppose — i → k

$P_{i\to k} = 1$

$E_i > E_k$

Now, with this background we know that we are looking we were looking at Ising model in equilibrium right. Now, think that these energy states that I was talking about those are the various energy states that the Ising model can access and at for at a particular value of energy corresponds to a certain number of micro-states you know different micro-states can have the same energy right. So, just think that this n i's are not particles, but the number of micro-states which are accessed at energy i, 3, 2, 1 and so on and so forth energy i.e, e 2, e 3, e 1 right.

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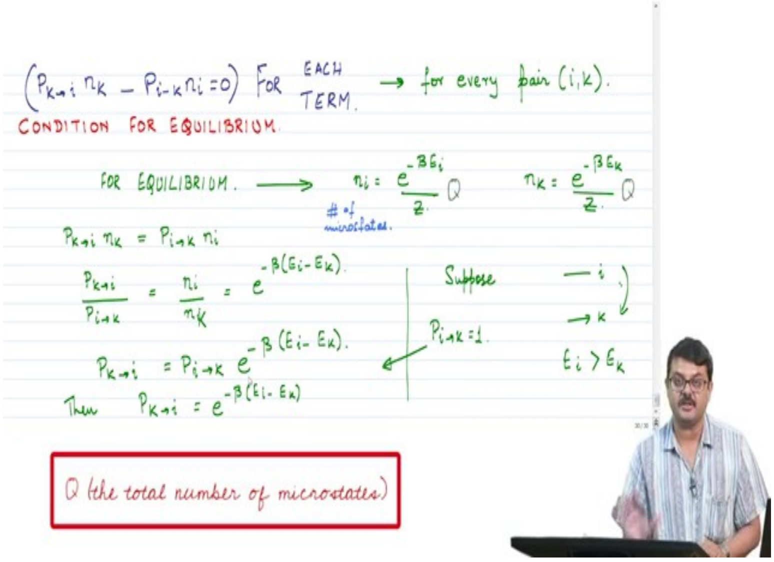

$(P_{k\to i} n_k - P_{i\to k} n_i = 0)$ FOR EACH TERM. → for every pair (i,k).

CONDITION FOR EQUILIBRIUM.

FOR EQUILIBRIUM. ⟶ $n_i = \frac{e^{-\beta E_i}}{Z} Q$ # of microstates. $n_k = \frac{e^{-\beta E_k}}{Z} Q$

$P_{k\to i} n_k = P_{i\to k} n_i$

$\frac{P_{k\to i}}{P_{i\to k}} = \frac{n_i}{n_k} = e^{-\beta(E_i - E_k)}$

$P_{k\to i} = P_{i\to k} e^{-\beta(E_i - E_k)}$

Then $P_{k\to i} = e^{-\beta(E_i - E_k)}$

Suppose — i → k

$P_{i\to k} = 1$

$E_i > E_k$

Q (the total number of microstates)

For equilibrium this relation holds and that relation holds for every energy state pair of energy states i and K. Now, we also know that the number of microstates which will be accessed. So, basically n i will be e to power minus beta E i by Z; n k will be e to the power minus beta E k by Z. So, higher energy microstates are accepted with are accessed with lower probability the basically normalizing constant is Z.

And, in that case we can write this to be we can rearrange this put in the expressions of n i and n k and we can write it; so, here there is a mistake there has been a mistake. So, now, I have corrected it and then this comes to be e to the minus beta E i minus E k is something like the Boltzmann factor; of course, the Boltzmann factor has to come here. And, then one can write P K i equal to P i K into e to the power minus beta E i by E K.

Now, suppose now suppose the particular K I am talking about is such that i is higher than K which means E i is has a higher value than E k right and if we set P i K equal to 1 then P K i automatically becomes a basically if you fix this value so, there are two unknowns here. So, we fix this value we immediately the value of this is fixed we can fix it to be 0.5 or 0.25 or 10 and then immediately the value of this gets fixed.

Here we have said let P i K equal to 1 and then P K i automatically gets fixed at this value which means that if i was at a higher energy if you basically say that if a micro-state is being accessed K which is of lower energy than i, accept the transition, accept the spin flip with probability 1, then between K and i the probability of accessing from going from K to i is this and that is exactly what we have implemented in our simulations and this relation holds for every pair of i's and K's right.

So, if it is going if this value is more I mean so, even if it was i plus 1 and K then basically you can again choose this that to be 1 right P i plus 1 to K to be 1 and then the probability of P K to i plus would suitably be affected right. So, this is where the metropolis algorithm comes from and this is the background physics is extremely important to know where the metropolis algorithm comes from. I intentionally discussed it at the end, so that you understood the algorithm.

With this I come to the end of this module and from the next class we will be discussing differential equations.

Thank you.