

**Numerical Methods and Simulation
Techniques for Scientists And Engineers
Saurabh Basu
Department of Physics
Indian Institute of Technology- Guwahati**

**Lecture 21
Applications of Importance Sampling in Statistical
Physics Ising Model and Phase Transitions**

So we will see one more example of important sampling in the, in the Monte Carlo technique that we have learned. And this time we are going to focus on statistical mechanics or statistical physics. And we will look at phase transitions and we leave out critical fundamental because that becomes too technical from the physics perspective. So, we just talked about phase transitions and how Monte Carlo in aids in seeing or demonstrating a phase transition.

So, as a prototype system will take an Ising model and will describe what an Ising model is. And so, phase transitions are really important things in condensed matter physics or statistical physics, where the system changes from one phase to another as function of the driving parameter, and that driving parameter could be anything which could be related to the you know the parameters of the Hamiltonian or it could be thermal effects, which is temperature, or it could be other things, you know, such as a bias voltage and things like that.

So, this study of phase transitions is always important and interesting, because the system changes from one phase to another. So let us take an example as the Ising model.

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Ising Model

- Ising model is a model of a magnet that shows a phase transition.
- The essential concept behind it (and true for other magnetic models as well) that bulk magnetism results from the contribution of magnetic dipole moments from many atomic spins.
- Ising model postulates a lattice (can be of any geometry, usually chosen as square in 2D and simple cubic in 3D) with a magnetic dipole or a spin on each site.

So what is an Ising model, so it is a model of a magnet or it shows magnetism and that also has a phase transition? So, it mainly shows a magnetic phase transition and that is what is being

used for the essential you know, idea, the premise behind it is that which is also true for many other magnetic models, such as Heisenberg model etc, that the bulk magnetism of any substance or any material, it results from the contribution of the magnetic dipole moments of many atomic spins coming from the constituents atoms or ions for that particular element or that particular material.

So, we are going to talk about magnetism and magnetism is coming from the magnetic dipole moments of the atomic spins. And this Ising model postulates a lattice and in principle this lattice could be of any geometry it could be in any dimension could be one dimension to dimension three dimension and so, on. And the geometry could be you know a linear chain in one dimension or a square lattice into dimension or cubic lattice in 3 dimension you can have a simple cubicle artist or you can have FCC face centered cubicle artist or a body centered cubic lattice in a two dimension one can have a honeycomb lattice or one can have you know other more complicated lattices such as Kagame etc and so on.

And with magnetic dipole or a spin located at each of these lattice sites, okay, so, suppose we are talking about a two dimensional square lattice, which is easy for us to demonstrate. So, these are the lattice sites the corners of weathers vertical and horizontal lines the intersect, so, these are the lattice points and here destroyed with a different colour there are spins which are pointing like will in principle in any direction.

But for Ising model will talk about only spins pointing up or down drawn a little, you know, out of the axis because just to show you the direction, but these are perfectly either pointing up or pointing down this is like a set component of any spin half object. And so, everywhere there is a spin of this kind and we want to see whether this has a finite magnetism and for that one has to postulate model or a model Hamiltonian.

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- The spins in the model are represented by scalar variables, s_i which can assume only two values ± 1 .
- They represent spins pointing in the up and down directions of unit magnitude.
- The interaction between these spins (which is the only term in the Hamiltonian) is between nearest neighbours.
- The Hamiltonian is written as,

$$H = -J \sum_{\langle i,j \rangle} s_i s_j - B \sum_i s_i$$

$\langle i,j \rangle$: nearest neighbours
 B : external magnetic field.

- J being positive makes the spins align in the same direction (up or down): Ferromagnet
- J being negative makes the neighbouring spins align in the opposite direction: Antiferromagnet
- One can calculate the partition function (Z) in closed form and calculate the average magnetisation using,

$$m = \langle s_i \rangle = \frac{1}{\beta} \frac{\partial \log Z}{\partial B_i}$$

$\beta = \frac{1}{k_B T}$ J & $k_B T$
 k_B : Boltzmann constant

- For a paramagnet $m = 0$; while for a magnetic system $m \neq 0$

And for the Ising model, the model Hamiltonian looks like here, just let us come to this in a while. So, these spins in this model are represented by scalar variables, which we call us S_i , which can assume only two values, namely plus one and minus one. Okay. So, they cannot take any other values. So, plus will correspond to say up and minus will correspond to down but that is just a convention, you can take your own convention to be just opposite of this convention.

So, the interaction between the spins and that being the only term in the Hamiltonian is between the nearest neighbour spins these spin variable S_i , so, it is S_i into S_j is the spin variable. So there is a sum over liquidated ij not put this sum over. So, these are some over i and these are, so when we write like this, these are nearest neighbours. Okay, and B 's is an external magnetic field. And this negative sign is simply conventional.

And the B can have either plus sign or minus sign, if it is a plus sign, then that would facilitate or rather that would, you know, promote that all the spins pointing in the same direction. So, either you have plus one into plus one, which will give you a plus one, or you can have a minus 1e into plus or minus 1, which will again give you a plus 1, so that the energy is minimized by the spins pointing in the same direction.

So, if it is between two neighbouring sides, that is true for all the neighbouring sites in the lattice. So, the essentially the oldest spins will be pointing up and one would had a ferromagnetism in this particular situation, if j is negative, then the it is energetically more favourable to have these neighbouring spins align in the opposite direction that is one being plus the other being minus in which case the product will be minus and hence this minus will multiply with this minus to give me sort of plus sign but then j being negative battle the minimize the energy.

So, that corresponds to an anti-ferromagnet, where the neighbouring spins are pointing in the opposite direction. And what one does or what one if one has gone through this statistical mechanics at the partial level or even at the rife level one knows that the thing to calculate is what is called is a partition function and usually we talk about the canonical partition function, which means that the system this system of n Ising on a lattice is connected to a bot of temperature T and this is given by;

So, so, the magnetization is given by the expectation value of the spins at a site i and this is written as $\frac{1}{\beta} \frac{\partial \ln Z}{\partial B_i}$ where Z is as said is the partition function it could be the canonical or the grand canonical partition function and it is kind of the derivative is taken with respect to the magnetic field at the site i and this would determine that whether the system is in a paramagnetic state, when m would be equal to zero that is there is no net magnetization of the system.

And therefore ferromagnetic system or for magnetic systems, so for example, in general, the value of m is not equal to 0. Okay, so this would tell us that whether we have a magnetic system or magnetised system or a non magnetic system, of course, if B is large, then you always have the all the spins pointing in the same direction as this external field. But most of the time, we want to talk about the spontaneous magnetism, that is the magnetization that one can have without this B term, so that the driving or rather the competition is between j and KT .

Where KT is the thermal energy, which will try to randomize, all the magnetic moments are the spins. And that will be done by the KT , which is a thermal energy and j is the magnetic term, which will try to align them given that j is positive and with a negative sign at the front. So we will have a magnetic system. Okay, so most of the time, we are interested in these spontaneous magnetization without the second term in the Hamiltonian.

But it could be there, and it poses no problem because it is a one body problem or one body term. And there is no problem in diagnosing the Hamiltonian even with this term being there.
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Role of Monte Carlo in computing correlations

- Usual goal in a Monte Carlo simulation is to compute expectation value of an observable (which could be the magnetization in trying to see magnetic phase transition from paramagnet at to a ferromagnet.
- Because we shall talk about systems in thermal equilibrium, temperature will always play an important role. In fact, $\frac{J}{k_B T}$.
- Think of a correlation, $\langle Q \rangle = \frac{\sum Q_i e^{-\beta E_i}}{\sum e^{-\beta E_i}}$, $i = 1 \dots M$ denote the states. M is the size of the sample.

So we essentially try to compute m okay. And this m is the magnetization as we have said, and this let us say the average monetization and things like that, okay. So, where is Monte Carlo coming into the picture and how do we get these Monte Carlo associated with this problem. So, usually goal in Monte Carlo simulation is to compute the expectation value of an observable that we have seen the expected value of the expectation value or just the expectation are various terms that are going for that as you go through literature they have different you know, nomenclature.

Now, this particular expectation value of an observable could be the magnetization, as we commonly know it, that this magnetization is an indicator of his transition, because if the magnetization vanishes, the system is safe to be in a para magnetic state. And if it is nonzero, then it is magnetised state or a magnetic state. And this is exactly what we have just discussed. And then we can have a feast transition as a function of the driving parameter from a magnet to a federal magnet, okay?

There is no act here, because we shall talk about the systems in thermal equilibrium, okay, because temperature any experiment that you can think of is not done at zero temperature is done at a finite temperature. So temperature will definitely play a role. Or rather, this ratio, as we have just said that this ratio will play a role, because if j very large compared to KT , then we have a magnetic system, as I said, could be ferromagnetic.

And if in the other limit if j is much smaller than KT , then we have a para magnetic system with no magnetic properties. Okay, so this ratio is very important in determining that whether the system has a federal magnetic property or para magnetic property and things like that. So just what we have written in the last page about this expectation value of S_i as being the spin

variable that has given site i , let us just talk about Q , any sort of quantity for which we want to calculate the correlation function or these expectation value.

And then what we have to do is that we have to take these Q_i and which is exponential minus beta E_i , E_i being the energy of the system, and i is not. So there is a bit of a sort of notational issue, this i is not a site index that we have said earlier. So what we can do is that we can change this if you like, to mn , and write this as $S_m S_n$, and maybe this as m , and then we can write this as S_m , okay.

Anyway, that is just so we know that these mn are actually these site indices of lattice could be in 3 dimensions or 2 dimensions as we have said or in any dimension and any lattice geometry. And so, this i rather would be the number of states that we are going to sample. And as we have said that these states are generated at random from certain distribution. And so this i is one to M where M denotes the number of states or, you know, I mean, basically M is the size of the sample or I mean sample means it is not the sample, it is not the material.

But it is the sample of the states or rather the number of states that we are going to consider from you know, arbitrary probability distribution. So, we have learned how to do these summations or integrals by using the Monte Carlo.

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- The (crude) Monte Carlo estimate of Q will be given by,

$$Q_M = \frac{\sum_i Q_i p_i e^{-\beta E_i}}{\sum_i p_i e^{-\beta E_i}}$$
- Q_M becomes more and more accurate as $M \rightarrow \infty$, i.e. $Q_M \rightarrow \langle Q \rangle$.
- Now the question is how does one choose the probability distribution p_i .
- The simplest choice is to pick all states with equal probability, i.e. uniform distribution.
- This will make

$$Q_M = \frac{\sum_i Q_i e^{-\beta E_i}}{\sum_i e^{-\beta E_i}} \quad \beta = \frac{1}{k_B T}$$
- From our experience, this must be a poor choice. Why?

So, the Monte Carlo crude or the simple as we have said, so crude and simple, the word crude seems a little crude, then you can use the word simple, the simple Monte Carlo estimate of key would be given by this, where Q_M , so this is equal to Q is replaced by or the expectation of Q is replaced by Q_M , which is equal to $Q_i P_i$ and an exponential minus beta E_i , okay. And divided by all these are some over i which are not appearing here, and P_i exponential minus beta E_i .

So, Q_m becomes more and more accurate if m goes to infinity, which means the sample of states that we are considering goes to very large values. But then as you know that we have a definite computational power. And we cannot go to any number of states to sample in physical computer. But this is true that if m goes to a very large value that is going to limit in the limit tending to infinity, your Q_m will give you the accurate estimate of this expectation of Q .

And if you are wondering what Q is, it could be anything for a given thermodynamics system. In this particular case, we are having magnetism in our mind. So, now the question is, how does, one choose the probability distribution, P_i , okay. And the simplest choice is, of course, to pick all states with equal probability, with no a priori assignment of probability. So I am completely unbiased. So it is a uniform distribution.

So this uniform distribution, we have seen that they are not very helpful, because there are too many of them one. And secondly, you do not know how to distinguish sort of the more important set states from the not so important ones. And particularly the problem is more important as we also going to come later is that since we are talking about low a temperature that is we are actually looking for the system to order as we tuned this j by KT , which means that j is larger than KT .

So we are in a limit of smaller temperature, it is only the system only, you know, spends more time or rather, mostly be found in a few states, among this large number of a plethora of states that we are having. So it is just only going to be reciting in these few states, which are only most important and the rest are not important and not contributing to this sum. So that tells you that if you take a random distribution, which means that equal distribution, uniform distribution with equal probability, then that P_i can be taken to be as one.

And then this Q_m reduces to a particularly simple form, which is Q_m equal to, again, this sum over i and exponential minus beta E_i . So just to remind you, every time that beta equal to one over KT , that is the convention that is used might have written it somewhere, but if not, then I will write it should have written it here. So beta is equal to 1 over KT , where K is called as the Boltzmann constant. And T the temperature in absolute scale. Okay. Alright, so we are with a uniform distribution, we have a have an expression for Q_m , which looks simple.

But of course, we know that from our experience that this must be a poor choice, because you are giving equal way to all states. Whereas all states are not really involved into this, sum, we have seen particular problem that the function as a value, which peaks around a certain value. So if you take a uniform distribution, you are really, you know, you have equal probability of

choosing points from the tail, which can cause which does not contribute much to the value of the integral, that is the one that we have seen in the last discussion.

So we know that this uniform distribution is rather poor choice, and perhaps something better should be done.

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- In an Ising model, a 3D cubic system of $10 \times 10 \times 10$ Ising spins would have 2^{1000} states $\approx 10^{300}$ states.
- A typical good computer sample upto 10^8 to 10^{10} states.
- So essentially one is sampling 1 in approximately 10^{290} states.
- The sum appearing in the expectation value at low temperature is dominated by a small number of states, with all the other states contributing very little.
- Thus by sampling only a small number of states, the hope to sample the important ones are very less.
- Hence Q_M will be a very bad estimate of $\langle Q \rangle$.
- Importance sampling comes to the rescue.

So let us just look at these, you know, the details of these simulation and implementation of the Monte Carlo. So in an Ising model, let us take a 3d cubic system, simple cubic system of 10 L equal to 10. So $10 \times 10 \times 10$, Ising space, which are 1000 spins, and each spin has two states, okay. So if you have two spins, one can have states which are like, up-up, or we can have up-down, or we can have down-up, or we can have down-down.

So these are 4 states, which is equal to 2^2 to the power 2 because we have 2 spins, we have to put the power to when you have n spins, so you have to do the power. And now since we have thousand spins $10 \times 10 \times 10$, which are arranged on a simple cubic lattice, left 2 to the power 1000 states, and that is a very, very large number. And that is a number which is close to 10^{300} states. So if you really have a sample 10^{300} states, that is no physical computer, available, even as today would be able to sample them.

And neither there is a need to do that. So at the; a typical good computer would, you know, do it up to something like 10^{10} states. So what happens is that you are leaving out to tend to the power 290 states from 10^{300} states. So, these, the sum that you are trying to calculate, which appears here, in this expression for Q_M is dominated by only a small number of states, the other states actually contribute very little.

But even those small number of states, you are going to miss because you are only you are going to miss a one in 10 to the power 290 states, and this is going to be a very bad approximation, because the ones that are dominantly contributing to the integral are being missed. And these are not, you know, helpful at all. So a Q_m will eventually give a very bad estimate of Q , okay.

And, and that is the reason that the important sampling comes to the rescue, okay. So, we are going to now use important sampling, and actually sample states which are accessible or achievable by a physical computer can sample and will have to only demarcate those states, and we have to have a rational behind that. So, we have learned important sampling, we just want to, you know, recapitulate it in this particular situation.

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Importance Sampling

- On the other hand if we had some ways of knowing which states could make important contributions to the sum above, we could pick them into our sample of M states and ignore all others. This is done by **importance sampling**.
- So our strategy would be instead of picking up M states in such a way that every state of the system is as likely to get chosen as any other.
- We pick them in such a way that the probability of a particular state i gets chosen with

$$p_i = \frac{1}{Z} e^{-\beta E_i}$$

Where $Z = \sum_i e^{-\beta E_i}$
- So that the Monte Carlo estimator takes a simple form

$$Q_M = \frac{1}{M} \sum_i Q_i$$

See that the complicate Boltzmann factors have cancelled out in the denominator.

So, we know that, on the other hand, if you have some ways of knowing which states could make important contributions to the sum above, we could pick them into our sample of m states and ignore all others; this is done by the important something, okay. So our strategy would be to, instead of picking up m states, randomly from a uniform distribution, we want that every state of the system.

So every state of the system is not as likely as any other state, rather, we pick them from a probability given by this one over z , and exponential minus beta i . So this is like some over i exponential minus beta i . So this is the probability that is going to be used not the probability one, which corresponds to a uniform distribution, you remember that we have used Gaussian or a normal probability distribution with some mean and variance for solving an integral that appeared in the last discussion.

In this particular case, that Gaussian distribution is replaced by this one, this distribution this B_i , where that is, as we have learned that z is called as the partition function of the system, which is sum over all states, all configurations, and exponential minus beta here. So the Monte Carlo estimated takes a particularly simple form, where Q_m equal to 1 over m , and sum over Q_i , and because all these Boltzmann factors that have completely cancelled each other, and you are left with only a Q_i .

And so this particular formalism or others, choice of this probability distribution entirely depends upon the problem and what has to use really common sense and looking at the integrand, or the function that needs to be integrated. And carefully and then decide on the probability distribution for doing the importance sampling. So this is the importance weight that we have learned in order to do this problem.

Okay, so Q_m really takes a form, which is 1 over m and sum over Q_i . And we have cancellation of these Boltzmann factors that are there.

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Markov Process

- The final question is that how exactly do we pick our states, so that each one appears with the correct Boltzmann probability.
- This is not a simple task. It is done by using a technique called as **Markov processes**. All Monte Carlo techniques rely on Markov process as the generating engine for the set of states to be used for calculating the expectation value.
- Markov process is a mechanism, which new state, v starting an old state μ with a transition probability $P(\mu \rightarrow v)$.
- For a true Markov process, the probability should satisfy:
 - A. They should not vary over time.
 - B. They should only depend on the properties of the states μ & v and no other states.
- Also

$$\sum P(\mu \rightarrow v) = 1$$

Now, the question is that how exactly do we pick our states? Okay, it is not only about the probability distribution, but for the reason that we will just see in a short while. So, we have to make a strategy for picking up the important states and as I said that at small temperature not all states are equally likely to contribute to the integral and there are a certain number of states that are important and one is to really know the technique in order to do that.

So, it is really not a simple task. And it is done by a technique which is called a Markov process. So, all Monte Carlo techniques really rely on this Markov processes as the generating engine for the state of states that are that will be used for computation of the expectation value

okay. So what is the Markov process the market processes a mechanism which a new state μ starting from an old state μ with a transition probability p going from μ to μ okay.

So, you have a state μ and you want to go to a state μ and there is certain probability for going towards that there is done by the metropolis algorithm will see that in a way, but this there is a probability and then from again from new one can go to another one called λ and from λ and other one to say χ and from χ to another state and so on. So, you actually depend or rather generate a sequence of states and these states are fairly independent from each other.

Because for a true Markov processes, it is written here, the probability should satisfy that they should not vary with time okay. So, over the time, these probabilities should remain constant, and they should only depend upon the properties of this pair of states μ and ν and no other states okay. So, this is very important that for the probability in going from μ to ν will depend upon the properties of these μ and ν states and no other states that are there in the ensemble.

And of course, the normalized probability should also be equal to one and this is a true for any for all states new the final states and this is a normalization of the probabilities okay.

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- In a Monte Carlo simulation, one uses the Markov process repeatedly to generate a Markov chain of states.
- Starting with a state μ , we use the process to generate a new state ν , and then use ν to generate another state λ and so on.
- The Markov process is chosen specially so that when it runs for long enough starting from a given state, it will eventually produce a succession of states which appear with probabilities given by the Boltzmann distribution.
- Reaching the Boltzmann distribution is equivalent to coming in thermal equilibrium.
- Without the Markov process, we would have chosen states at random with probabilities proportional to $e^{-\beta E_i}$.
- This would more disastrous than our crude Monte Carlo, as we shall land up rejecting virtually all states, since the probabilities for their acceptance are exponentially small.

So, in a Monte Carlo simulation, one uses the Markov processes these processes that repeatedly to generate a Markov chain of states this is what exactly I was saying, starting with a μ , we use the process to generate a new state μ and then use ν to generate another state λ and then proceed in this particular manner to generate a large number of Markov states.

So the Markov processes chosen specially when it runs, I mean, when it runs for a long enough time, starting from a given initial state, it will eventually produce a succession of states which appear with the probabilities given by the Boltzmann distribution, okay. So, reaching the Boltzmann distribution is equivalent to coming to thermal equilibrium for a particular case.

So, as you generate more and more Markov chains or rather states in the Markov chain, what happens is that you are likely to reach an equilibrium which is called as a thermal equilibrium or is called as the Boltzmann distribution. And so, what happens is that the particular utility of this Markov process, without the Markov process, we would have chosen states with at random with probabilities, which are given by or proportional to exponential minus beta E_i , E_i being the energy of that particular state, or that configuration. And this actually would have been more, you know, disastrous compared to even simple minded Monte-Carlo. And we would have actually land up rejecting virtually all states, because the probabilities for their acceptance were exponentially small. Okay. So just without the Markov process, if we have gone ahead and use this probability, we would have virtually left out all states, because any particular state would come with exponential small probability, and that would have served no purpose.

Okay, that would have been even worse than actually calculating the whole in the Monte Carlo estimate with a uniform distribution.

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Details of the simulation

- Start with a random configuration of spins in a $L \times L \times L (= N)$ spins. For this one can choose a random number generator $[0: 1]$ and multiply by N (approximate it to the nearest integer to identify the spins on the lattice).
- To produce a Markov sequence, use another random number generator so that a particular spin is picked up, say, s_i . Call this configuration as μ .
- Flip that spin (from $\uparrow \rightarrow \downarrow$ or $\downarrow \rightarrow \uparrow$). Call this new configuration as ν .
- Calculate the change in energy according to the Hamiltonian, $E_\mu - E_\nu$.
- Define the difference as, $E_{\mu\nu} = E_\mu - E_\nu$.

So let us quickly go through the details of the simulation. So we wish to start from a random configuration of spins in L cross L cross L system, which is equal to N spins and L being the, you know, the lateral dimension of the lattice. So we have assembled cubicle artists consisting

of L cube number of spins. So for this one can generate a random number from 0 to one and multiply that by n , which is equal to LQ and approximated to the nearest integer to identify the spins in the on the lattice.

So okay, so this is, this is a bit, alright, so what we mean to say is that you want to identify sites in the lattice, and that you want to do randomly, so what you do is that you either you run identify estate by this method, or a side by this method, rather, it is a site in that lattice by this method, and then you occupy it via either an upstream or downstream, okay. And to produce a Markov sequence, if you use another random number generator, so that a particular spin is picked up, say S_i , and this call this configuration mean, okay.

So, you start with a random configuration of spins by generating a random number where spins are, you know, you say that between 0 and 1e, if it is less than .5, I will put down spin and if it is greater than .5, I will put on up spin and things like that. So randomly in the lattice, you have put up and down spins, then you need to generate a Markov sequence your generator, okay. And for that, you pick another random number, okay, use another random number generator, and call that.

So identify your spin by that random number generator by multiplying it by N and approximating dating to the nearest integer, call this particular configuration, as μ , add μ means the initial configuration, now flip the spin from if the spin is initially up, then flip it to down, or if it is initially down, then flip it to up and call this new configuration as μ . Okay. So you have an old configuration μ which has from a given random distribution of spins on lattice you have generated that.

Now you have identified one spin, and have caused the flip, call this new one as new, the new status or configuration as μ , calculate the change in energy according to the Hamiltonian. So Hamiltonian is just writing down the Ising term, it is $S_i S_j$ with the ij . So you calculate the energy of the changing energy of the Hamiltonian, E_μ , and $E_{\mu'}$, $E_\mu - E_{\mu'}$. So let us call that $E_{\mu\mu'}$ is $E_\mu - E_{\mu'}$. And so this difference is defined as this.

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- The $E_{\mu\nu}$ will decide whether the move (i.e. flipping the spin is acceptable)
 - a) If $E_{\mu\nu}$ is negative or zero, we accept the move.
 - b) If $E_{\mu\nu}$ is positive, we draw another random number x and check whether,
 - i. if $e^{-\beta E_{\mu\nu}} \geq x$: Accept the move
 - ii. if $e^{-\beta E_{\mu\nu}} \leq x$: Reject the move

Repeat this procedure several times by forming a long trajectory in the configuration space. This is known as **Metropolis algorithm**.

This is roughly the simulation details. Expected value of magnetisation is computed so as to demonstrate the phenomena of Phase transition.

And now, this $E_{\mu\nu}$ will decide whether the move is acceptable or not acceptable. Okay, so this flipping of spin is acceptable or not. And so we define certain conditions that if $E_{\mu\nu}$ is negative, that is because of this flip, the energy is minimized, and we accept the move immediately without any further condition. Now, even if $E_{\mu\nu}$ is positive, we draw another random number x , and check whether the exponential minus beta, $E_{\mu\nu}$ is greater than x , then if you then you accept the move.

And if it is less than, so this should be less than instead of this will, so this is not, if you have a greater than equal to then of course, you accept the move, if it is less than, then you reject the move, okay, you cannot have both greater than equal to and less than equal to. Now repeat this procedure several times by forming a long trajectory in the configuration space. So what I mean to say is that you identify another spin, do the same procedure, and see that accept the move or reject the move, go to another spin.

And you again, pick up a random number, identify your spin, flip it, see whether the move is acceptable according to this condition, and things like that. So we actually generate a long trajectory of these systems in the configuration space. And this is precisely called as a Metropolis algorithm. There are more things which are our Ergodicity and so on, I will not go into details, but what our motive is to explain that these Monte Carlo simulations are particularly very important for a variety of situations including, you know, simple computation of simple integrals to very complicated cases such as this as the phase transition and things like that.

So, this is roughly the simulation details, the expected value of the magnetization is computed so as to demonstrate the phenomena of phase transition. So after the thermalization after the

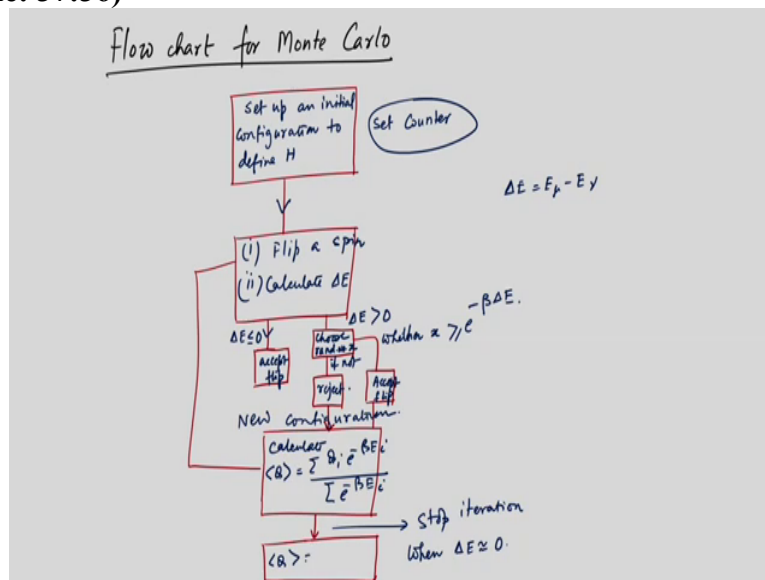
thing, the system has achieved the equilibrium or the Boltzmann distribution, the thermal equilibrium so to say, then, you calculate the magnetization and see that if the magnetization is has a finite value and large value so to say, so that we can see that the system is magnetic.

And if it is either zero or very small, then we will have to see that it is a non magnetic system or poorly magnetic system, and so on. So, if you have a varying parameters a temperature or or that j over KT , then there is a particular TC that one can achieve TC is the transition temperature, so, one can identify a transition temperature in a given system. And this is from a para magnet to ferro magnet, this transition temperature is called a quire temperature.

Incidentally, in one dimension, the system has no transition, that is the transitions are only at T equal to you know zero, which means that there is no ordering temperature finite ordering temperature. And the reason is simple. The reason is that the energy difference between the demagnetized states of the para magnetic states and the magnetic states is only by just breaking one bond. And that is a one over N effect.

So if N is large, that effect is very small. And then you always have a disordered system or a para magnetic system, accepting at equal to 0, which is not a physical reality. Okay, so these are precisely where they are applied. Let me show you an algorithm which we make things a little more clear.

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So it is a flow chart for Monte Carlo. So we will have so this I am just drawing the boxes and then we will write what are the steps and things like that. So this and okay and then there are just give me a minute to finish this drawing. So set up all right an initial configuration to define H and you can set a counter here okay. Then you come to this one, and then you say that flip a

spin and calculate the ΔE which is $\Delta E = E_{\mu} - E_{\nu}$, if ΔE is less than or equal to 0 then you accept flip which we have said.

If ΔE greater than 0 then choose random number x okay then you see that whether x , x is greater than or equal to $\exp(-\beta \Delta E)$ if that is the case then you accept the move accept flip, flip if not reject the flip and one actually goes to a new configuration. So, then you calculate Q which is equal to you know sum over all these states and then Q_n or Q_i whatever we have written earlier.

$Q_i = \exp(-\beta E_i)$ divided by $\sum \exp(-\beta E_i)$ and so on and stop iterations when ΔE becomes almost equal to 0, which means that the system is not iterating and the system has reached an equilibrium and then by flipping farther spins, the energy of the system is not changing. So, that is the equilibrium that we are talking about the thermal equilibrium that we are talking about and then of course, use this Q which is equal to $1/m$.

Sum over Q_i from 1 to m and then use this thing to calculate the expectation value of the quantity that you are interested in as we have told several times that this could be the magnetization and the magnetization being nonzero would indicate that the system has gone into a ferromagnetic state okay. And one can do this in one dimension and one does not find any phase transition which means that there is no finite temperature at which or other this j by KT is not you know at any.

So, this only happens at T equal to 0 which means the value of this ratio to be infinity or a but in two and three dimensions, there are finite temperatures that was the phase transition occur, okay. So, we have seen very elaborately the utility and the versatile nature of this Monte Carlo simulation. And these are very important, you know, simulation tools that are accepted by the computational community.

Both in you know, various branches of science and engineering. The good thing is that, you know, a lot of things one does not really need to know and it depends upon some distribution, which is more preferred than other the distribution. So, these are important sampling, the important sampling is a very important step in improving the accuracy of this Monte Carlo method, we shall stop here and with this discussion on the Monte Carlo and we will proceed with another simulation in the next discussion.