

# The Monte Carlo Method of Random Sampling in Statistical Physics

<sup>1</sup>Akabuogu E. U., <sup>2</sup>Chiemeka I. U. and <sup>3</sup>Dike C. O.  
*Department of Physics, Abia State University, Uturu, Nigeria.*

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**Abstract:** *The Monte Carlo technique of random sampling was reviewed in this work. It plays an important role in Statistical Mechanics as well as in scientific computation especially when problems have a vast phase space. The purpose of this paper is to review a general method, suitable to fast electronic computing machines, for calculating the properties of any system which may be considered as composed of interacting particles. Concepts such as phase transition, the Ising model, ergodicity, simple sampling, Metropolis algorithm, quantum Monte Carlo and Non-Boltzmann sampling were discussed. The applications of Monte Carlo method in other areas of study aside Statistical Physics were also mentioned.*

**Keywords:** *Ising Model, Phase transition, Metropolis algorithm, Quantum Monte Carlo, Observables, Non-Boltzmann Sampling.*

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## I. Introduction

In Statistical Mechanics, many real systems can be considered: These systems can be broadly divided into two namely:

- Systems which are composed of particles that do not interact with each other, therefore uncorrelated. These model are called Ideal gases
- Systems which consist of particles which interact with each other such that interparticle interactions cause correlation between the many particles. Such systems therefore exhibit phase transition. A typical example of such system is the Ising model.

For such many particle systems, systematic exploration of all possible fluctuations is often a very complicated task due to the huge number of microscopic states that must be considered and the cumbersome detail needed to characterize these states. However, there have been formulated a number of practical methods for sampling relevant fluctuation for non-interacting systems: the fluctuations can be handled by the Factorization and the Born-Oppenheimer approximation. For the interacting systems, which involve phase transition (e.g the Ising model), the Monte Carlo Method (MCM) and the Molecular Dynamic (MD) method can be employed to estimate the fluctuations (Chandler, 1987).

The goal of statistical mechanics is to understand and interpret the measurable properties in terms of the properties of their constituent particles and the interactions between them. This is done by connecting thermodynamic function to quantum-mechanical equations. The two central quantities being the Boltzmann factor and the partition function. The ability to make macroscopic predictions based on microscopic properties is the main advantage of statistical mechanics. For problem where the phase space dimensions is very large – this is especially the case when the dimension of phase space depends on the number of degrees of freedom – the Monte Carlo Method outperforms any other integration scheme. The difficulty lies in smartly choosing the random samples to minimize the numerical effort.

The Monte Carlo method in computational physics is possibly the most important numerical approaches to study problems spanning all unthinkable scientific discipline. These include, all physical sciences, Engineering, computational biology, telecommunication, finance and banking etc. The idea is seemingly simple: Randomly sample volume in d-dimensional space to obtain an estimate of an integral at the expense of an experimental error (Helmut, 2011).

In this work, focus will be on the application of Monte Carlo Method to canonical systems with coupled degrees of freedom such as the Ising model. The theory of phase transition will be quickly revisited while the Ising model will be used as a representation of our interacting many particle systems. The simple sampling and the Metropolis sampling will be treated as a Monte Carlo Method. In addition, quantum extensions of the Monte Carlo Method such as the ‘Quantum Monte Carlo and the Path Integral method’ will be discussed. The non- Boltzmann sampling and the application of the Monte Carlo Method in other area of study aside statistical physics will also be outlined.

## II. Theory of Phase Transition

Monte Carlo method is hugely employed in systems with inter-particle interactions: Phase transition is a clear manifestation of such interactions. Many processes in life exhibit phase transition. A good example being

the solid to liquid, liquid to gas and the reverse changes due to the effect of temperature and/or pressure. A phase change of great importance, which is frequently used in statistical mechanics, is that of magnetic systems. Ferromagnets are clear example of such magnetic system. A ferromagnet is a material that exhibit spontaneous magnetization. In ferromagnets, magnetic ions in the material align to create zero magnetism. Each ion exerts a force on the surrounding ions to align with it. An aligned state is a low energy state while entropy increases at higher temperature to cause substantial alignment. When these individual interactions build up to a macro scale, alignments produce a net magnetism. If there is a sudden change in magnetism at a certain temperature, we say that there is a phase transition (Eva, 2010).

### III. The Ising Model

Once the electrons spin was discovered, it was clear that the magnetism should be due to large number of electrons spinning in the same direction. A spinning charged particle has a magnetic moment associated with it. It was natural to ask how the electrons all know which direction to spin, because the electrons on one side of a magnet do not directly interact with the electrons on the other side. They can only influence their neighbors. The Ising model was designed to investigate whether a large fraction of the electron could be made to spin in the same direction using only local force (Wikipedia).

The idealized simple model of a ferromagnet is based upon the concept of interacting spins on an unchanging lattices is called the Ising model. It is named after the physicist Ernst Ising. The model consists of a discrete variable that represents magnetic dipole moments of atomic spins  $S_i$  that can be in one state (+1 or -1).

$$S_i \begin{cases} +1 & \text{represents "spinup"} \quad \uparrow \\ -1 & \text{represents "spin down"} \quad \downarrow \end{cases}$$

The spins are arranged in a graph usually a lattice, allowing each spin to interact with its neighbors. The model allows the identification of phase transitions, as a simplified model of reality. The one – dimensional model has no phase transition and was solved by Ising in 1925; the 2- dimensional model was solved by Lans Onsager (Binder *et al*, 1992).

In the Ising model, we consider a system of N spins arranged on a lattice as illustrated in fig 1 below.

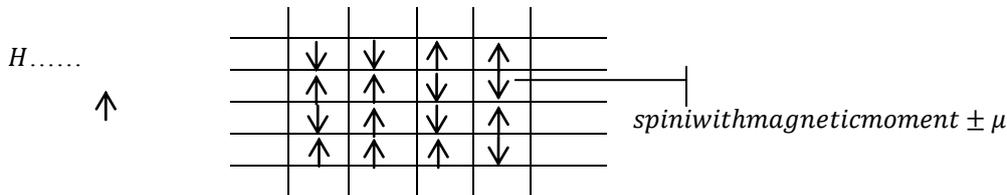


Fig 1: An Ising model

In the presence of a magnetic field  $H$ , the energy of the system in a particular state,  $v$  is

$$E_v = - \underbrace{\sum_{i=1}^N H \mu s_i}_{\text{external magnetic energy}} - \underbrace{j \sum_{ij} s_i s_j}_{\text{energy due to interaction of the spin}} \quad (1)$$

where  $j$  is the coupling constant.

The spin at each lattice site (i) interact with its four nearest neighbor sites such that the overall Hamiltonian for the system is

$$H = -j \sum_{ij} s_i s_j \quad (2)$$

Where the sum over  $\langle ij \rangle$  represents a sum over the nearest neighbors of all the lattice sites.

By setting up a system obeying this Hamiltonian, we can find the mean energy,  $\bar{E}$  and the specific heat,  $C$ , per spin for the Ising ferromagnet from

$$\bar{E} = \frac{\frac{1}{N} \sum_i E_i e^{-\beta E_i}}{Z} \quad (3)$$

And

$$C = \frac{\sigma_{\bar{E}}^2}{NK_B T} \quad (4)$$

We can also estimate the mean magnetization,  $\bar{M}$ , from the following ensemble average

$$\bar{M} = \frac{1}{N} \sum_i s_i \quad (5)$$

As also noted by Frenkelet *al* (1996), we are interested in the variations of these quantities with temperature as this system will undergo a phase change and so discontinuities should appear in its macroscopic properties at a

particular value  $T$ . It should be possible to compare the behavior of  $[E], C, [\bar{M}]$  and also the partition function,  $Z(\beta)$  with the result in the literature to determine if the simulation is giving a reasonable result.

#### IV. Phase Change Behavior of the Ising Model

The difference between the thermal energy available  $K_B T$ , and the interaction exchange energy ( $J$ ) defines the behavior of the Ising model. At high temperature  $T > T_c$ , when the thermal energy is much greater than the interaction energy, the interaction energy will be drowned out by randomizing effect of the heat bath and so the patterns of the spins on the mesh will be random and there will be no overall magnetization. However, as the temperature is lowered, ( $T < T_c$ ), and ( $J > 0$ ), the correlation between the spin begin to take effect. Lower temperature allows clusters of like spins to form, the size of which defines the correlation length ( $\epsilon$ ) of the system, therefore it may be anticipated that for low enough temperature, the stabilization will lead to cooperation phenomenon called Spontaneous Magnetization: that is through interactions between nearest neighbors, a given magnetic moment can influence the alignment of spins that are separated from the given spin by a macroscopic distance. These long ranged correlations between spins are associated with long ranged order in which the lattice has a net magnetization even in the absence of a magnetic field. The magnetization

$$\langle M \rangle = \sum_{i=1}^N \mu S_i \tag{6}$$

In the absence of the external magnetic field  $H$ , is called the spontaneous magnetization (Chandler, 1987).

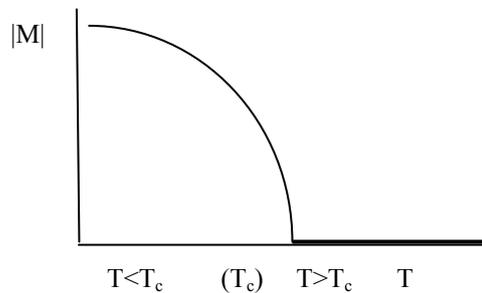


Fig 2: Plot of magnetization against temperature of an Ising model.

As shown in fig. 2,  $T_c$  (the Curie temperature or critical temperature) denote the highest temperature to which there can be non – zero magnetization, we expect that after the critical point, the system must make a decision as which direction is favoured, until at  $T=0$  all spins are pointing either upwards or downwards. Both choices are energetically equivalent and there is no pre-guess which one the system will choose. The breaking of symmetry, such having to choose the favoured direction for the spins and divergence of system parameter such as  $\epsilon$  and  $C$  are characteristics of the phase change (Binder *et al*, 1992).

Chandler (1987) opined that the conditions at which all spins align in either upward or downward direction (at  $T < T_c$ ) and when all the spin are randomly aligned (at  $T > T_c$ ) can be considered or modelled as a phase change transition between a ferromagnetic and paramagnetic conditions of the magnetic system. The 1 – and – 2 – Dimensional Ising model is as shown in fig. 3.

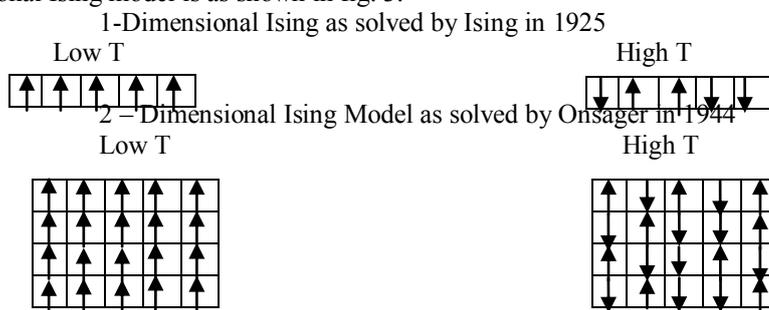


Fig 3: 1 – and – 2 – Dimensional Ising models

As the temperature increases, entropy increase but net magnetization decreases. This alignment and misalignment of spin constitute a phase change in an Ising model.

#### V. Variables describing the system

According to Laetitia (2004), if we consider a lattice of  $N^2$  spins which has 2 possible states, up and down, In order to avoid the end effects, periodic boundary conditions are imposed. The equilibrium of the system can be

- Magnetization,  $M = \frac{1}{N^2} S$  (7)

- HeatCapacity,  $C = \frac{1}{N^2} \left(\frac{1}{KT}\right)^2 ((E^2) - \langle E \rangle^2)$  (8)

It is linked to the variance of the energy.

- Susceptibility,  $\chi = \frac{1}{N^2} \frac{1}{KT} ((S^2) - \langle S \rangle^2)$  (9)

It is linked to the variance of the magnetization

### VI. Expected behaviour of the system

The free energy satisfies

$$F = -K_B T \ln Z = \langle E \rangle - TS \quad (10)$$

Where  $Z = \sum_{\alpha_j} e^{-\beta E(\alpha_j)}$

The system approaches the equilibrium by minimizing F (the free energy). At low temperature, the interaction between the spins seem to be strong, the spins tend to align with another. In this case, the magnetization reaches its maximal value  $|M| = 1$  according its formula, the magnetization exists even if there is no external magnetic field. At high temperature, the interaction is weak, the spins are randomly up or down, as such the magnetization is close to the value  $|M| = 0$ . Several configuration suits; the system is metastable.

The magnetization disappears at a given temperature. There exists thus a transition phase. In zero external magnetic fields, the critical temperature is the Curie temperature  $T_c = \frac{2}{\ln(1+\sqrt{2})}$  (obtained by Onsager's theory).

According to the transition phase theory, the second-order derivative of the free energy in  $\beta$  &  $T$  are discontinuous at the transition phase, as the susceptibility and the heat capacity are expressed with these derivatives, they should diverge at critical temperature.

### VII. The Monte Carlo Method

With the advent and wide availability of powerful computers, the methodology of computer simulation has become a ubiquitous tool in the study of many body systems. The basic idea in these methods is that with a computer, one may follow the trajectory of system involving  $10^2$  or even  $10^3$  degrees of freedom. If the system is appropriately constructed – that is, if physically meaningful and boundary conditions and interparticle interactions are employed – the trajectory will serve to simulate the behaviour of a real assembly of particles and the statistical analysis of the trajectory will determine meaningful predictions for the properties of the assembly. The importance of these methods is that, in principle they provide exact results for the Hamiltonian under investigation. These simulations provide indispensable benchmarks for approximate treatment of non-trivial systems composed of interacting particles (Chandler, 1987).

There are 2 general classes of simulations: One is called the Molecular Dynamic method (MD); Here one considers a classical dynamic model for atoms and molecules, and there trajectory is formed by integrating Newton's equations of motion. The other class is called the Monte Carlo method (MCM). This procedure is more generally applicable than molecular dynamics in that it can be used to study quantum systems and lattice models as well as classical assemblies of molecules. As a representative of a non-trivial system of interacting particles, we choose the Ising magnet to show how the Monte Carlo method can be applied.

The term Monte Carlo method was coined in 1940's by physicists, S. Ulam, E. Fermi, J. Von Neumann and N. Metropolis (amongst others) working on the nuclear weapon project at Los Alamos National Laboratory. Because random numbers (similar to processes occurring at in a casino, such as the Monte Carlo casino in Monaco) are needed, it is believed that, that was the source of the name. For problems where the phase space dimensions is very large – this is especially the case when the dimension of phase space depends on the number of degrees of freedom – the Monte Carlo method outperforms any other integration scheme. The difficulty lies in smartly choosing the random samples to minimize the numerical effort (Helmut, 2011). The Ising model can often be difficult to evaluate numerically, if there are many states in the system. Consider an Ising model with L lattice sites. Let

- $L = |\Lambda|$ : the total number of sites on the lattice
- $\alpha_j \in \{-1, +1\}$ : an individual spins site on the lattice,  $j = 1, \dots, L$ .
- $S \in \{-1, +1\}$ : state of the system

Since every spin has  $\pm spin$ , there are  $2^L$  different states that are possible. This motivates the reason for the Ising model to be simulated using the Monte Carlo method. As an example, for a small 2-dimensional Ising magnet with only  $20 \times 20 = 400$  spins, the total number of configuration is  $2^{400}$ . Yet Monte Carlo procedures routinely treat such system successfully sampling only  $10^6$  configurations. The reason is that Monte Carlo schemes are

devised in such a way that the trajectory probes primarily those states that are statistically most important. The vast majority of the  $2^{400}$  states are of such high energy that they have negligible weight in the Boltzmann distribution (wikipedia). The Monte Carlo technique works by taking the random sample of points from phase space, and then using that data to find the overall behaviour of the system. This is analogous to the idea of an opinion poll. When trying to work on the opinion of the general public on a particular issue, holding a referendum on the subject is costly and time consuming. Instead, we ask a randomly sampled proportion of the population and use the average of their opinion as representation of the opinion of the whole country. This is much easier than asking everybody, but is not as reliable. We must ensure that the people asked are chosen truly at random (to avoid correlations between the opinions), and be aware of how accurate we can expect our results to be given that we are only asking a relatively small number of people. Issues as these all are analogous to the implementation of the Monte Carlo technique (Frenkel, 1997). To carry out a Monte Carlo method on an Ising, an  $N^2$ -array is initialized at a low temperature with aligned spins (this is called a cold start) or at a high temperature with random values 1 or -1 (this is called the hot start). The Monte Carlo method consists to choose randomly a spin to flip. The chosen spin is flipped, if it is favourable for the energy. When the energy becomes stable, the system reached the thermalisation, then configurations are determined by the Metropolis Algorithm in order to determine the properties of interest as the heat capacity and the susceptibility.

In statistical physics, expectation values of quantities such as the energy, magnetisation, specific heat etc – generally called ‘observables’ – are computed by performing a trace over the partition function  $Z$ . Within the canonical ensemble (where the temperature  $T$  is fixed), the ‘expectation value or thermal average of an observable,  $A$  is given by

$$\langle A \rangle = \sum_s P_{eq}(s) A_s \tag{11}$$

Where  $s$  denotes a state,  $A_s$  is the value of  $A$  in the state  $s$ .  $P_{eq}(s)$  is the equilibrium Boltzmann distribution.

$$\langle A \rangle = \frac{1}{Z} \sum A_{(s)} e^{-\beta E_{(s)}} \tag{12}$$

Represent the sum overall states  $S$  in the system and  $\beta = \frac{1}{KT}$  where  $K$  is the Boltzmann constant.  $Z = \sum_s \exp[-\beta E_{(s)}]$  is the partition function which normalises the equilibrium Boltzmann distribution. It is good to note that the Boltzmann factor  $P_i \propto e^{-\beta E_i}$  is not a probability until it has been normalised by a partition function. Such that the true nature of the equilibrium Boltzmann distribution  $P_{eq}(s)$  is

$$P_{eq}(s) = \frac{e^{-\beta E_{(s)}}}{\sum_s e^{-\beta E_{(s)}}} \tag{13}$$

One can show that the free energy,  $F$  is given by

$$F = -kT \ln Z \tag{14}$$

All thermodynamic quantities can be computed directly from the partition function and expressed as derivatives of the free energy. Because the partition function is closely related to the Boltzmann distribution. It follows that we can ‘sample’ observables with states generated according to the corresponding Boltzmann distribution. A simple Monte Carlo algorithm can be used to produce such estimate (Newmann *et al*, 1999).

### VIII. Simple Sampling

The randomly most basic sampling technique consists of just randomly choosing points from anywhere within the configuration space. A large number of spins patterns are generated at random (for the whole mesh) and the average energy and magnetization is calculated from data. However, this technique needs to suffer from exactly the same problems as the quadrature approach, often sampling from unimportant areas of the phase space. The chances of a randomly created array of spin producing an all – up/ all- down spin pattern is remote ( $\sim 2^{-N}$ ), and high temperature random spin array is much likely. The most common way to avoid this problem is by using the Metropolis Importance Sampling, which works by applying weights to the microstates.

### IX. The Metropolis Sampling

The algorithm first chooses selection probabilities  $g(\mu, \nu)$ , which represents the probability that state  $\nu$  is selected by the algorithm out of all states given that we are in state  $\mu$ . It then uses acceptance probabilities  $A(\mu, \nu)$  so that detailed balance is satisfied. If the new state  $\nu$  is accepted, then we move to that state and repeat with selecting a new state and deciding to accept it. If  $\nu$  is not accepted, then we stay in  $\mu$ . The process is repeated until some stopping criteria is met, which for the Ising model is often when the lattice becomes ferromagnetic, meaning all of the sites point in the same direction (Frenkel *et al*, 1996).

We implementing the algorithm, we must ensure that  $g(\mu, \nu)$  is selected such that ergodicity is met (by this we mean that orbit of the representative point in phase space goes through all points on the surface). In thermal equilibrium, a system’s energy only fluctuates within a small range. With this knowledge, the concept of single-spin flip dynamics – which states that in each transition, we will only change one of the spin sites on the lattice. Furthermore, by using a single-spin flip dynamics, we can get from one state to any other state by

flipping each site that differs between the 2 states one at a time. The random choices for the spins performed with the aid of the ‘pseudo – random number generator’ – an algorithm that generates a long sequence of random numbers uniformly distributed in the interval between 0 and 1- commonly available with digital computers.

Having picked out a spin at random, we next consider the new configuration  $\nu$ , generated from the old configuration,  $\mu$ , by flipping the randomly identified spin  $\mu$ . The change in configuration changes the energy of the system by the amount

$$\Delta E_{\mu\nu} = E_\nu - E_\mu \tag{15}$$

Chandler (1987) opined that this energy difference governs the relative probability of configurations through the Boltzmann distribution, and we can build this probability into the Monte Carlo trajectory by criterion for accepting and rejecting moves to new configuration. The maximum amount of change between the energy of this present  $E_\mu$  and any possible new state’s energy  $E_\nu$  is  $2J$  between the spin we choose to ‘flip’ to move to the new state and that spin’s neighbour.

Specifically for the Ising model, implementing the single-spin flip dynamics, we can establish the following:

- Since there are  $L$  total sites on the lattice, using the single – spin as the only way we transition to another state, we can see that there are a total of  $L$  new state  $\nu$  from our present state  $\mu$ . Detailed balance tells us that the following equations must hold:

$$A(\mu, \nu)P_\beta(\mu) = A(\nu, \mu)P_\beta(\nu) \tag{16}$$

Such that,

$$\frac{P(\mu, \nu)}{P(\nu, \mu)} = \frac{g(\mu, \nu)A(\mu, \nu)}{g(\nu, \mu)A(\nu, \mu)} = \frac{A(\mu, \nu)}{A(\nu, \mu)} = \frac{P_\beta(\nu)}{P_\beta(\mu)} = \frac{e^{-\beta(E_\nu)/Z}}{e^{-\beta(E_\mu)/Z}} = e^{-\beta(E_\nu - E_\mu)} \tag{17}$$

Where  $P_\beta(\nu)$  is the transition probability for the next state  $\nu$ , and it only depends on the present state  $\mu$ . Thus we want to select the acceptance probability for our algorithm to satisfy

$$\frac{A(\mu, \nu)}{A(\nu, \mu)} = e^{-\beta(E_\nu - E_\mu)} \tag{18}$$

If  $E_\nu > E_\mu$ , then  $A(\nu, \mu) > A(\mu, \nu)$ .

By this reasoning, the acceptance algorithm is

$$A(\mu, \nu) = \begin{cases} e^{-\beta(E_\nu - E_\mu)} & \text{if } E_\nu > E_\mu \\ 1 & E_\nu \leq E_\mu \end{cases}$$

Conclusively, the basis for the algorithm is as follows

- Pick a spin site using the selection probability  $g(\mu, \nu)$  and calculate the contribution of the energy involving the spin.
- Flip the value of the spin and calculate the new contribution.
- If the new energy is less, keep the flipped value i.e. if  $E_\nu \leq E_\mu$ , we accept the move
- If the new energy is more, only keep the probability  $e^{-\beta(E_\nu - E_\mu)}$ .
- Repeat: we now repeat this procedure for making millions of steps thus forming a long trajectory through the configuration space.

This process is repeated until the stopping criteria is met, which for the Ising model is often when the lattice have become ferromagnetic (at low energies  $T < T_c$ ), meaning that all the sites point in the same direction(Wikipedia).

### X. Practical Implementation of the Metropolis Algorithm

A pseudo – code Monte Carlo program to compute an observable  $\vartheta$  for the Ising model is the following:

```

1  algorithm using_metropolis A (T, steps)
2  initialize starting configuration  $\mu$ 
3  Initialize  $\varrho = 0$ 
4
5  for (counter = 1 .....steps) do
6  generate trial state  $\nu$ 
7  compute  $p(\mu \rightarrow \nu, T)$ 
8   $x = \text{rand}(0,1)$ 
9  If( $p > x$ ) then
10     Accept  $\nu$ 
11  fi
    
```

```

12
13  ρ += ρ(ν)
14    done
15
16  return ρ/steps

```

After initialization, in line 6 a proposed state is generated by e.g. flipping a spin. The energy of the new state is computed and henceforth the transition probability between states  $P = T(\mu \rightarrow \nu)$ . A uniform random number  $X \in [0,1]$  is generated. If the probability is larger than the number, the move is accepted. If the energy is lowered  $\Delta E > 0$ , the spin is always flipped. Otherwise the spin is flipped with a probability  $P$ . Once the new state is accepted, we measure a given observable and record its value to perform the thermal average at a given temperature. For steps  $\rightarrow \infty$  the average of the observable converges to the exact value, again with an error inversely proportional to the square root of the number of steps. In order to obtain a correct estimate of an observable, it is imperative to ensure that one is actually sampling an equilibrium state. Because in general, the initial configuration of the simulation can be chosen at random – population choices being random or polarized configuration - the system will have to evolve for several Monte Carlo steps before an equilibrium state at a given temperature is obtained. The time  $\tau_{eq}$  until the system is in thermal equilibrium is called ‘equilibrium time’, it depends directly on the system size and it increases with decreasing temperatures. In general, it is a measure on ‘Monte Carlo Sweeps’ i.e. 1 MCS=N spin updates. In practice, all measures observables should be monitored as a function of MCS to ensure that the system is in thermal equilibrium. Some observables such as energy equilibrates faster than the others (e.g. Magnetization) and thus equilibration time of all observables measured need to be considered. It is expected that a plot of the variables when averaged over a partition function, shows discontinuities at a particular temperature (Helmut, 2011).

### XI. The Non – Boltzmann Sampling

According to Mezei (1987), the success of Monte Carlo is based on its ability to restrict the sample of the configuration space to the extremely small fractions that contributes significantly to most properties of interest. However, for calculating free energy difference, adequate sampling of a much larger subspace is required. Also for the related problems of potential of mean force calculations, the structural parameter along with the potential of mean force are calculated and has to be sampled uniformly. These goals can be achieved by performing the calculation using an appropriately modified potential energy function  $V$  or  $E_v^{(0)}$ . Specifically, Non Boltzmann is used in cases where one need to

- Sample part of the phase space relevant for a particular property
- Complete simulation when sampling of a specific region of the configuration space is required that may not be sampled adequately in a direct Boltzmann sampling. The technique calls for sampling with a modified potential
- Sample phase space more efficiently.

Suppose it is convenient to generate a Monte Carlo trajectory for a system with energy  $E_v^{(0)}$ , but you are interested in the averages for a system with a different energetic.

$$E_v = E_v^{(0)} + \Delta E_v \quad (19)$$

For example, suppose we wanted to analyse a generalized Ising model with couplings between certain non – nearest neighbours as well as nearest neighbours. The convenient trajectory might then correspond to that for the simple Ising magnet, and  $\Delta E_v$  would then be the sum of all non-nearest-neighbours interaction. How might we proceed to evaluate the average of interest from the convenient trajectories?

Chandler(1987) suggested that the answer is obtained from a factorization of the Boltzmann factor:

$$e^{-\beta E_v} = e^{-\beta E_v^{(0)}} e^{-\beta \Delta E_v} \quad (20)$$

With this simple property, we have

$$Q = \sum_v e^{-\beta E_v} = \frac{Q_0 \sum_v e^{-\beta E_v^{(0)}} e^{-\beta \Delta E_v}}{Q_0} \quad (21)$$

$$= Q_0 \langle e^{-\beta \Delta E_v} \rangle_0 \quad (22)$$

Where  $\langle \dots \dots \rangle_0$  indicates the canonical ensemble average taken with energetic  $E_v^{(0)}$ . A similar result due to the factorization of the Boltzmann factor is

$$\langle G \rangle = Q^{-1} \sum_v G_v e^{-\beta E_v} \quad (23)$$

$$= (Q_0/Q) \langle e^{-\beta \Delta E_v} \rangle_0 \quad (24)$$

$$= \langle G_v e^{-\beta \Delta E_v} \rangle_0 / \langle e^{-\beta \Delta E_v} \rangle_0 \quad (25)$$

The formula provides a basis for Monte Carlo procedures called the ‘non-Boltzmann sampling’ and ‘the Umbrella sampling’. In particular, since a Metropolis Monte Carlo trajectory with energy  $E_v^{(0)}$  can be used to

compute the averages denoted by  $\langle \dots \dots \rangle_0$ , we can use the factorization formulas to compute  $\langle G \rangle$  and  $\langle Q/Q_0 \rangle$  even though the sampling employing  $E_v^{(0)}$  is not consistent with the Boltzmann distribution  $\exp(-\beta E_v)$ .

Non – Boltzmann sampling can also be useful in removing bottlenecks that create quasi-ergodic problems and in focussing attention on rare events. Consider the former first, suppose a large activation barrier separates one region of configuration space from another, and suppose this barrier can be identified and located at a configuration or sets of configurations. We can then form a reference system in which the barrier has been removed: that is, we take

$$E_v^{(0)} = E_v - V_v \tag{26}$$

Where  $V_v$  is large in the region where  $E_v$  has the barrier and it is zero otherwise. Trajectories based upon the energy  $E_v^{(0)}$  will indeed waste time in the barrier region, but they will also pass one side of the barrier to the other thus providing scheme for solving problems of quasi-ergodicity.

Also an example of the latter occurs when we are interested in a relatively rare event. For example, suppose we want to analyze the behaviour of surrounding spins given that an  $n \times n$  block were all perfectly aligned. While such blocks do form spontaneously and their existence might catalyze something of interest, the natural occurrence of this perfectly aligned  $n \times n$  block might be very infrequent during the course of the Monte Carlo trajectory. To obtain a meaningful statistics from these rare events, without wasting time with irrelevant though accessible configurations, we have to perform a non-Boltzmann the Monte Carlo trajectory with energy like:

$$E_v^{(0)} = E_v + W_v \tag{27}$$

Where  $W_v$  is zero for the interesting class of configurations, and for all others  $W_v$  is large. The energy  $W_v$  is then called an Umbrella potential. It biases the Monte Carlo trajectory to sample only the rare configurations of interest. The non – Boltzmann sampling performed this way is called the umbrella Sampling (Chandler, 1987).

## XII. Quantum Monte Carlo

In addition to the aforementioned Monte Carlo Methods that treat classical problems, quantum extensions such as variational Monte Carlo, Path Integral Monte Carlo etc have been developed for quantum systems. In quantum Monte Carlo simulation, the goal is to avoid considering the full Hilbert space, but randomly sample the most relevant degree of freedom and try to extract the quantities of interest such as the Magnetization by averaging over a stochastic process.

According to Chandler (1987), to pursue this goal, we first need to establish a framework in which we can interpret quantum-mechanical observables in terms of classical probabilities. The process is called ‘quantum-classical’ mapping and it allows us to reformulate quantum many-body problems in terms of models from classical statistical mechanics, albeit in higher dimensions. To achieve this ‘quantum classical mapping’ and carry out a quantum Monte Carlo, the concept of ‘discretized quantum paths’ will be followed. In this representation, quantum mechanics is Isomorphic with the Boltzmann weighted sampling of fluctuations in a discretized classical systems with many degrees of freedoms. Such sampling can be done by Monte Carlo and thus this mapping provides a basis for performing quantum Monte Carlo calculations.

Many Monte Carlo sampling schemes exist that can be used to generate numerical solutions to Schrodinger equation. To illustrate the Quantum Monte Carlo simulation, we will focus on one – ‘path integral Monte Carlo’ which is popularly used to study quantum systems at non-zero temperatures.

As an example, one can look at a simple one model: the two-state quantum system coupled to a Gaussian fluctuating field. It is a system that can be analyzed analytically and comparison of the exact analytical treatment with the quantum Monte Carlo procedure serves as a useful illustration if the convergence of Monte Carlo sampling.

The quantal fluctuations of the model are to be sampled from the distribution

$$W(u_1, \dots, u_p; \xi) \propto \exp[\mathcal{S}(u_1, \dots, u_p; \xi)], \tag{28}$$

Where

$$\begin{aligned} \mathcal{S} &= -\frac{\beta \xi^2}{2\sigma} + (\beta/P)\mu \sum_{i=1}^P u_i \xi \\ &= \frac{1}{2} \ln(\beta \Delta/P) \sum_{i=1}^P u_i u_{i+1}. \end{aligned} \tag{29}$$

$$\text{Here } u_i = \pm 1 \tag{31}$$

specifies the state of the quantum system at  $i$ th point on the quantum path, there are  $P$  such points, the parameters  $\mu$  and  $\Delta$  correspond to the magnitude of the dipole and half the tunnel splitting of the two-state system, respectively. The electric field,  $\xi$ , is a continuous variable that fluctuates between  $-\infty$  and  $+\infty$ , but due to the finite of  $\sigma$ , the values of  $\xi$  close to  $\sqrt{\sigma/\beta}$  in magnitude are quite common.

The quantity  $\mathcal{S}$  is often called the action. It is a function of the  $P$  points on the quantum path  $(u_1, \dots, u_p)$ . The discretized representation of the quantum path becomes exact in the continuum limit of an infinite number of points on the path- that is,  $P \rightarrow \infty$ . In that limit, the path changes from a set of  $P$  variables,  $u_1$  to  $u_p$ , to a function of a continuous variable. The action is then a quantity whose value depends upon a function, and such a quantity is called a functional.

Consequently, a computer program can be written in BASIC to run on an IBMPC. Such program, samples the discretized weight function  $W(u_1, \dots, u_p; \xi)$  by the following procedure:

- Begin with a configuration
- One of the  $P+1$  variables  $u_1$  through  $u_p$  and  $\xi$  is identified at random, and the identified variable is changed. For instance, if the variable is  $u_1$  the change corresponds to  $u_1 \rightarrow -u_1$ . If on the other hand, the identified variable is the field  $\xi \rightarrow \xi + \Delta\xi$ , where the size of  $\Delta\xi$  is taken at random from a continuous set of numbers generated with aid of the 'pseudorandom-number generator'
- This change in one of the variables causes a change in the action  $\Delta\mathcal{S}$ . For example, if  $u_i \rightarrow -u_i$  then  $\Delta\mathcal{S} = \mathcal{S}(u_1, \dots, -u_i, \dots, \xi) - \mathcal{S}(u_1, \dots, u_i, \dots, \xi)$
- The Boltzmann factor associated with this change,  $\exp(\Delta\mathcal{S})$ , then compared with a random number  $x$  taken from the uniform distribution between 0 to 1.
- If  $\exp(\Delta\mathcal{S}) > x$ , the move is accepted.
- If however  $\exp(\Delta\mathcal{S}) < x$  the move is rejected.

An accepted move means that the new configuration of the system is the changed configuration. A rejected move means that the new configuration is unchanged from the previous one.

As with the Ising model, this standard Metropolis procedure for a Monte Carlo step is repeated over and over again producing a trajectory that samples configuration space according to the statistical weight  $W(u_1, \dots, u_p; \xi)$ . Typical results are then being obtained by averaging properties over these trajectories. A particular example of such results is the 'solvation energy' corresponding to the average of the coupling between the electric field and the quantal dipole, that is

$$E_{solv} = \left\langle \frac{1}{p} \sum_{i=1}^p \mu_i \xi \mu_i \right\rangle \quad (32)$$

### XIII. Conclusion

The Monte Carlo method of random sampling was reviewed in this work. It works by taking the random sample of points from phase space, and then using the data to find the overall behaviour of the system. To carry out this method on interacting systems, an array is initialized at a low or high temperature; spins are chosen randomly to flip. The chosen spin is flipped if it satisfies the boundary condition that is favourable to the energy. Expectation values of the Observables such as the energy, magnetization, specific heat etc are computed by performing a trace over the partition function,  $Z$ . The Monte Carlo applied to the Ising model which describes the properties of materials allows obtaining the thermodynamic quantities variations. For such model, when the Monte Carlo method is carried out, it is expected that

- Without magnetic field, a phase transition at the critical temperature is strongly marked. This transition separates  $T < T_c$ , where the magnetization is maximum, the spins are aligned, and  $T > T_c$  where the magnetization is in order of zero, the spins are randomly oriented.
- In the presence of magnetic field, the phase transition is not so marked. At a very high temperature, the field has no effect because of the thermal agitation. In a general way, the spins align with the magnetic field but at  $T < T_c$  the changes of direction happen only if field is above a critical value.

The use of the Monte Carlo stretches beyond statistical mechanics as its use is seen in Engineering, telecommunication, biology etc.

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