Stochastic Project: Monte Carlo simulations of the 2D Ising Model

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Abstract

The simplest theoretical description of ferromagnetism is called the Ising model. This model was invented by Wilhelm Lenz in 1920: it is named after Ernst Ising, a student of Lenz who chose the model as the subject of his doctoral dissertation in 1925.
The aim of this project is introduce an Ising model and investigate the properties of a two dimensional ferromagnet with respect to its magnetization and energy at varying temperatures. The observable are evaluated as an application of Monte Carlo techniques. Key background is given about the relevance and effectiveness of this stochastic approach and in particular the applicability of the Metropolis-Hastings algorithm in *FORTRAN* programming language.

1 Introduction

1.1 Background

Ferromagnetic are a class of materials that can retain magnetization in absence of an external magnetic field. Such materials exhibit long-range ordering on an atomic level resulting in formation of domains areas where unpaired electrons have identical spins.

In non-magnetized materials domains with opposite alignments cancel each other's fields out, but through exposure to an external magnetic field nonzero net magnetization can be achieved.

At high temperatures thermal motion competes with the tendency for dipoles to align. When the temperature is raised to a point called the Curie temperature, the system can no longer sustain spontaneous magnetization and a second-order phase transition occurs.

1.2 Square-Lattice 2D Ising Model

Consider Λ is a 2-dimensional lattice of spins in a magnetic field of strength H, with a linear space of L, each spin has 4 neighbors and is subject to the magnetic force. If we assume it only interacts with its nearest neighbors (not the diagonals), we find the Hamiltonian of this system to be:

$$H(\sigma) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \quad i,j \in \Lambda, \quad J > 0 \qquad (1)$$

where J is the strength of interaction between the 2 spins, and $\sigma = \{\sigma_i,\ i \in \Lambda\}$ denotes a $configuration$ of spins on Λ, with $\sigma_i = \pm 1$. The sum $\langle i,j \rangle$ runs over the nearest neighbours of i.
The nature of the interaction in the model is contained in the sign of the interaction coupling constant J. If J is positive it means that the material has a ferromagnetic nature (parallel alignment) while a negative sign would imply that the material is antiferromagentic. The relative

positioning of nearest neighbours of spins is shown in Figure 1.

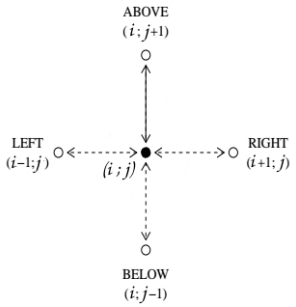


Figure 1: positioning of nearest neighbours of spins

Solving this problem consists in finding the transfer matrix of this distribution. This will allow predicting how will the spins in this system change when some parameters change.
The 2D Ising model undergoes a phase transition at the inverse critical temperature (in the thermodynamic limit):

$$\beta_c = \frac{ln(1) + \sqrt{2}}{2J} \tag{2}$$

For $\beta > \beta_c$ the ising model exhibits a spontaneous magnetization:

$$m_\beta = \left[1 - \frac{1}{\sinh^4(2)}\right]^{\frac{1}{8}} \tag{3}$$

In this simulation the dimension of the grid will be considered 100×100 $(L = 100)$ and $k_B = J = 1$ as consequence in this case $T_c = \beta_c^{-1} \approx 2.269$, time is measured in number of sweeps $N = L^2$ (Sampling every N time), at temperature range from 1 to 4.
Also a periodic boundary conditions was used with the following initial configurations $\{\sigma_i\}$:

i. $\sigma = +1$ (Positive initial configurations).

ii. $\sigma = -1$ (Negative initial configurations).

iii. $\sigma = \pm 1$ (Random initial configurations "with probability 50%").

1.3 Metropolis Monte Carlo Method

A Monte Carlo calculation is defined, as explicitly using random varieties and a stochastic process is characterized by a random process that develops with time. From what we have established with regards to the sampling being analogous to a time averaging along a stochastic trajectory in the phase space it is possible to simulated this process by using the Monte Carlo method. The algorithm used is design around the principle of the Metropolis sampling.
Let G is a graph with vertex set V and edge set E denoted by $\langle i, j \rangle$

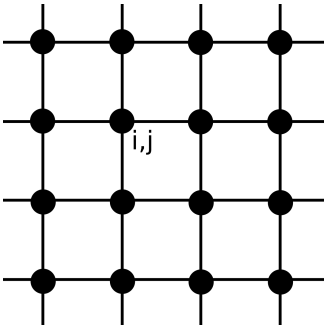


Figure 2: Vertex set V with edge set E

on each vertex i we introduce random variable called span σ_i which take values $\{-1, +1\}$, the vector spins $\vec{\sigma}(\sigma_1, \sigma_2, ..., \sigma_{|V|})$ is the "$state$" or $configuration$ of spins the entire system, where $|V| = N = L^2$. $V = [0, L^2] \cap \mathbb{Z}$ and E - the edges joining nearest neighbors of V.
Using a simple random walk on the Ising model lattice, the Metropolis algorithm is as following:

1. Initiate the grid with one of initial conditions.
2. Calculate the system energy H_α.
3. Pick a random spin $\{\sigma_k\}$.
4. Try to flip it: $\sigma_{ij} := -\sigma_{ij}$.
5. Calculate the energy change ΔH according to this flip.

$$\Delta H = H_{new} - H_\alpha \tag{4}$$

   (a) If $\Delta H < 0$, accept the flip.

   (b) If $\Delta H > 0$, accept with probability π_β,

$$\pi_\beta = e^{-\frac{\Delta H}{K_B T}} \tag{5}$$

      i. Generate a random number $a \in [0, 1]$

      ii. Accept if $\pi_\beta > a$

6. When a trial gets rejected, the spin is put back: $\sigma_{ij} := -\sigma_{ij}$
7. If the highest possible number of iterations has not been reached yet, go to 2.

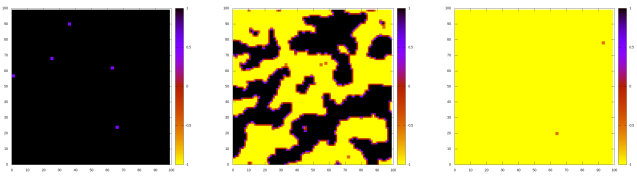
Listing 1: Metropolis Function FORTRAN Code

```
Do u = 1, Ittdy
!=|1|= Pick a random spin ==================
    CALL RANDOM_NUMBER(r)
    Rand = INT(r * l) + 1
    UN = Neighbors(l, Rand(1), Rand(2))

!=|2|= Local Energy Change Calculation ====
    dEnergy = (V(UN(1),Rand(2)) + V(UN(2),Rand(2)) + V(Rand(1),UN(3))  + V(Rand(1),UN(4)))
    dEnergy = 2 * dEnergy * V(Rand(1),Rand(2))

!=|3|= Calculate The Probability ==========
    PiPr = EXP(-(1/T) * dEnergy)
    CALL RANDOM_NUMBER(Rnd)

!=|4|= Energy Change Acceptance ===========
    IF ((dEnergy < =0) .OR. (PiPr >= Rnd)) THEN
       V(Rand(1),Rand(2)) = - V(Rand(1),Rand(2))

!=|5|= Calculate New Energy And Mag =======
       Mag = Mag + 2 * V(Rand(1),Rand(2))
       En = En + dEnergy
    END IF
END DO
```

2 Results

After implementing the algorithm the result was as following:

2.1 Initial Configuration Effect



(a) (b) (c)

Figure 4: Different initial configurations for T = 1
(a) Positive i.c., (b) Random i.c.,
(c) Negative i.c.

Figure 3 shows the different initial configurations for the grid, as a black color represents the value of (1) and yellow color for (-1).
In the figure 5 and 6 is displaying time dependence of energy and magnetization per spin at $T = 1$ with different configurations.
A speed convergence can be observed in case of positive (green line) and negative (red line) configurations, on another hand for random configuration need more time to reach convergence also the convergence can tends to the nearest stable configuration at that temperature (positive or negative configuration).

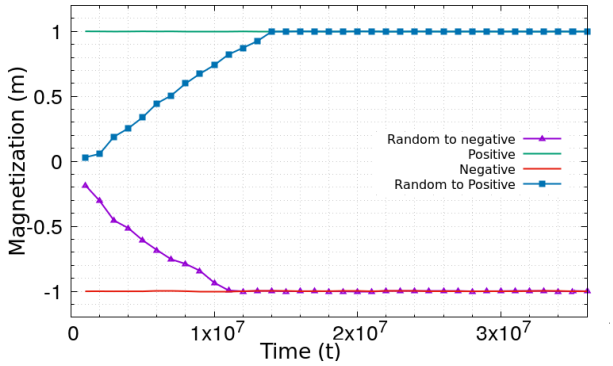


Figure 5: Magnetization per spin development with time

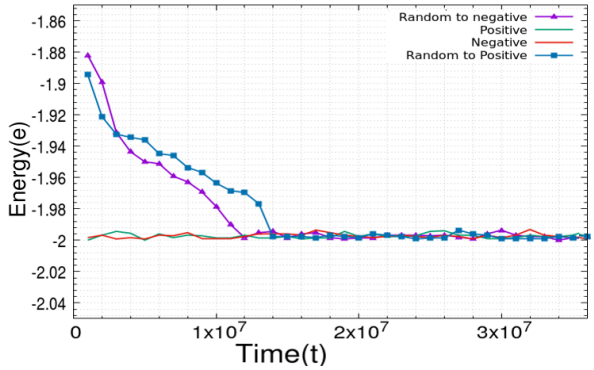


Figure 6: Energy per spin development with time

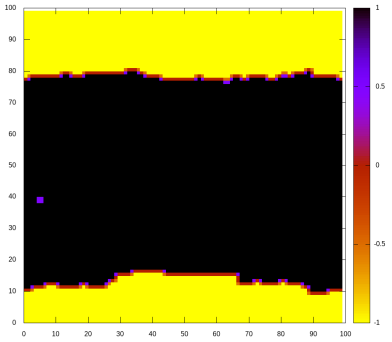
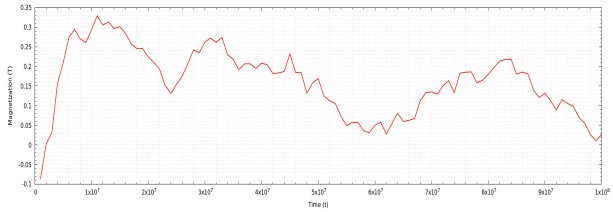
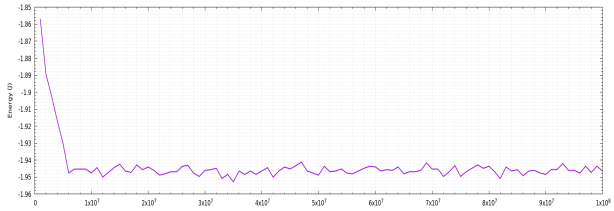


Figure 7: Unstable configuration

It worth to mention that in some random configurations, the simulation shows instability after reaching to a certain arrangement of elements, it may need larger time of simulation but this always happens when a thick line of opposite configuration appear horizontally or vertically in the grid.



(a) Magnetization per spin development with time



(b) Energy per spin development with time

Figure 8: instability after 10^8 of running time

This instability may be referred to that the system reached to the minimum possible energy which is clearly appeared in figure 8 and the system already achieved to energy stability so any change in configuration will be faced by rejecting.

2.2 Temperature increment

After a few steps after the initial temperature some samples was collected at $T = 2$ and $T = 2.5$ for all simulations (for P i.c, N i.c and Random i.c.) and the results was interesting.

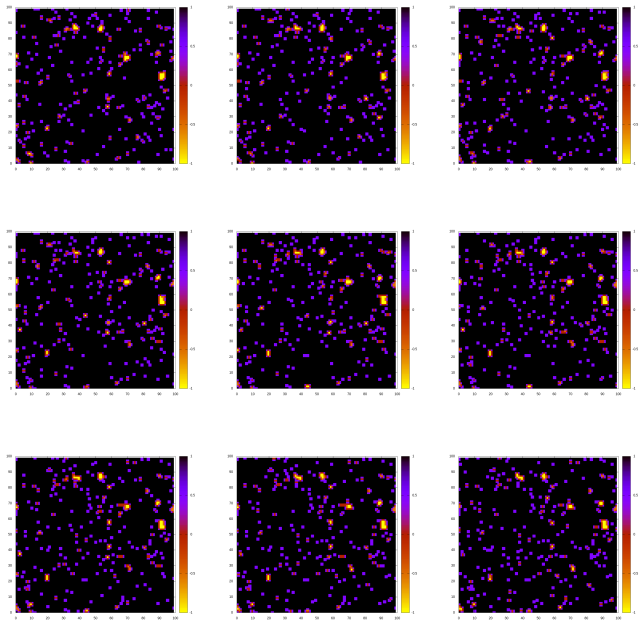


Figure 9: Microscopic configurations sampled at different times with positive i.c. for $T = 2$

For $T = 2$ most of spins are positive (The initial configuration remains without changing) That's because in a low temperature most of spins tends to be aligned, with the lowest energy for the system so changing spins is rare. Therefore, the lattice sticks to the initial condition as a ferromagnetic material.

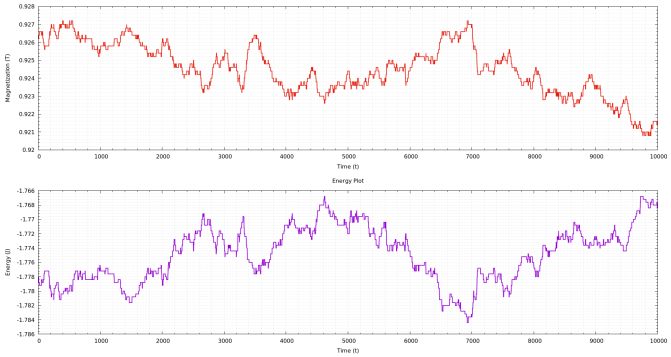


Figure 10: Magnetization (red line) and Energy (violet line) per spin variation with time showing a small change $T = 2$

On another hand, at temperature $T = 2.5$ a different behaviour was noted as the number of apposite spins seems equal and resulting configurations appear random disordered. as the energy of the system increased due to the temperature the spend tends to spin as paramagnetic material.

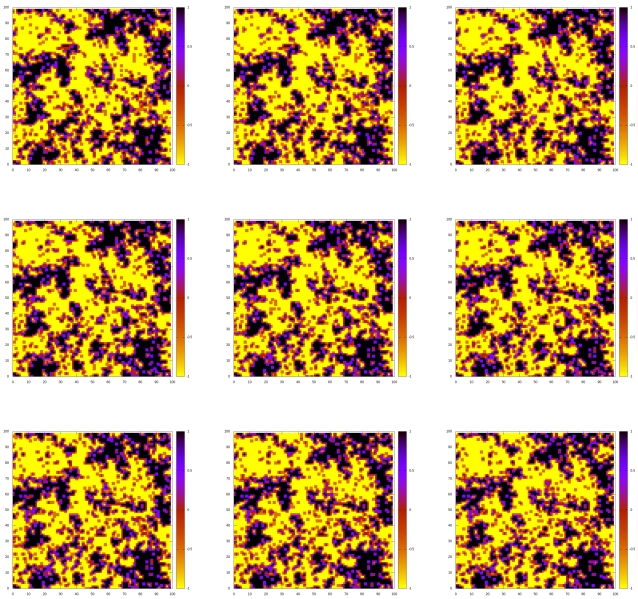


Figure 11: Microscopic configurations sampled at different times with positive i.c. for $T = 2.5$

Also the range of oscillation in the higher temperature is bigger and the time needed before start sampling is larger, This is due to the fact that in ferromagnetic regime spins in the lattice tends to align which keep the lowest energy for the system, but in the case of paramagnetic regime spins change their values a lot due to the high energy, therefore variables also oscillate more.

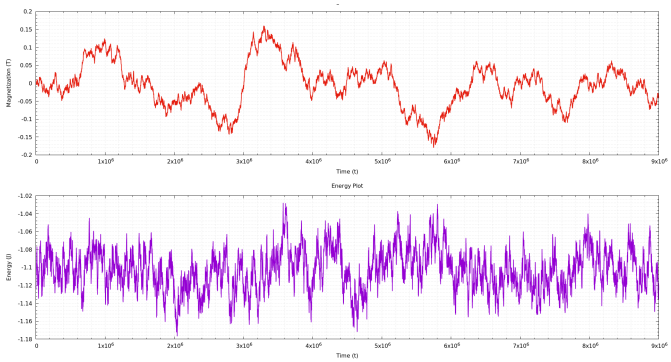


Figure 12: Magnetization (red line) and Energy (violet line) per spin variation with time showing a high range of changing $T = 2.5$

The same in case of negative initial configuration but with opposite configuration in $T = 2$ as the system resist against any change.

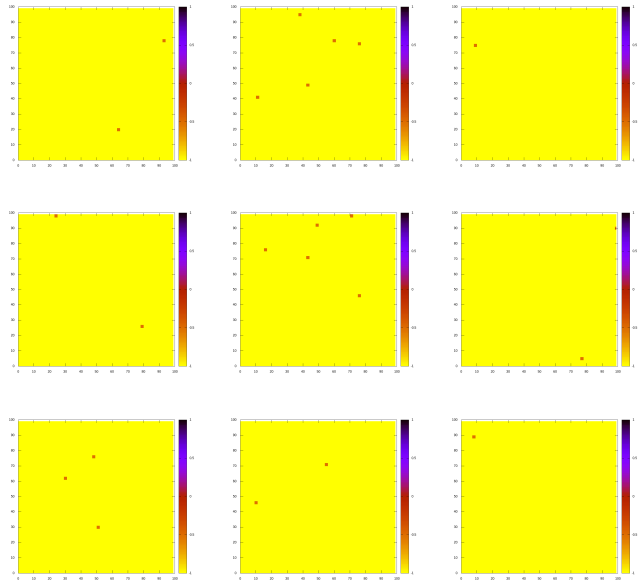


Figure 13: Microscopic configurations sampled at different times with Negative i.c. for $T = 2$

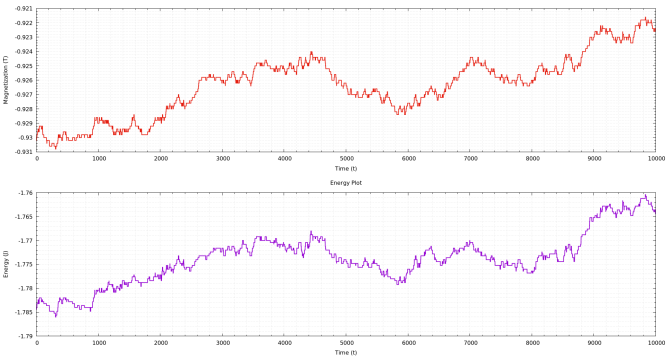


Figure 14: Magnetization (red line) and Energy (violet line) per spin variation with time showing a small change for $T = 2$

Also in the random initial configuration case after reaching stability as shown in previous subsection, It is behaves according to the reached configuration (either positive " + 1" or negative " − 1") then as same as above the configuration tends to to be aligned in the low temperatures and tends to change randomly in case of high temperatures.

Noteworthy this behaviour is called *Themalization* as the process of physical bodies reaching thermal equilibrium through mutual interaction. In general the natural tendency of a system is towards a state of equipartition of energy and uniform temperature that maximizes the system's entropy.

2.3 Magnetization and the susceptibility

The program that was implemented for this discussion started at a temperature of $T = 1$ and progressively stepped up in temperature to $T = 4$ with intervals of $\delta T = 0.1$ (60 temperature points).

One hundred million (10^8) Monte Carlo steps (mcs) per spin where used in order to ensure a large sample of data to average over (10^4) *samples*(N).

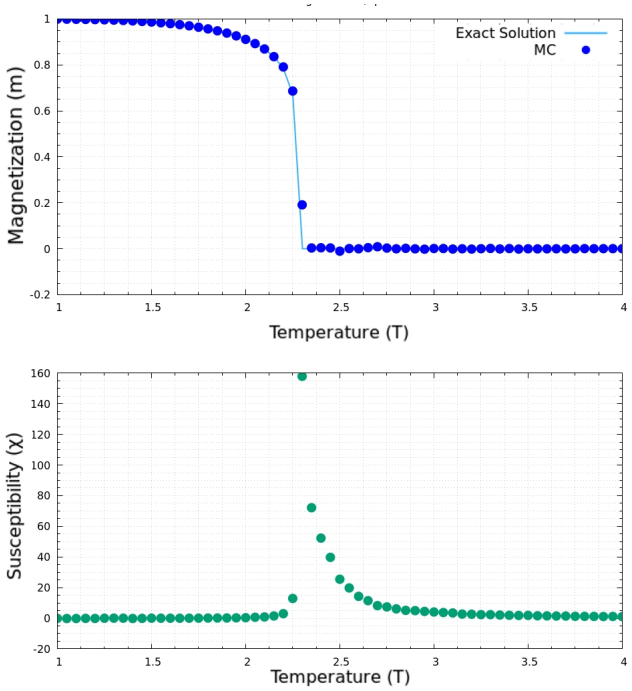


Figure 15: (a) Mean Magnetization (blue points) and (b) Magnetic Susceptibility (green points) both developing with temperature

The susceptibility is a measure of how much a material will become magnetized in an applied magnetic field and can be expressed by:

$$\chi = \frac{\partial M}{\partial S} \tag{6}$$

where M is the magnetization and S is the magnetic field strength.
The behaviour of the magnetization at high and low temperature are as the theory (random to stable parallel aligned configuration).but at the critical temperature a sudden configuration change happened that leads the susceptibility to be tended to infinity. this is shown clearly in figure 15

The susceptibility that is produced in our data is thus not exactly equivalent to the theoretical susceptibility χ, and we will be distinguished as χ'. The scaling characteristic of this susceptibility is, however, equivalent to the theoretical value.

$$\chi' = \beta N(\langle m^2 \rangle) - \langle m \rangle^2) \tag{7}$$

The physical variables calculated:

$$\langle m \rangle = \frac{1}{N}\sum_{i=1}^{N} \sigma_i \quad and \quad \langle m^2 \rangle = \frac{1}{N}\sum_{i=1}^{N} \sigma_i^2$$

2.4 Energy and the specific heat

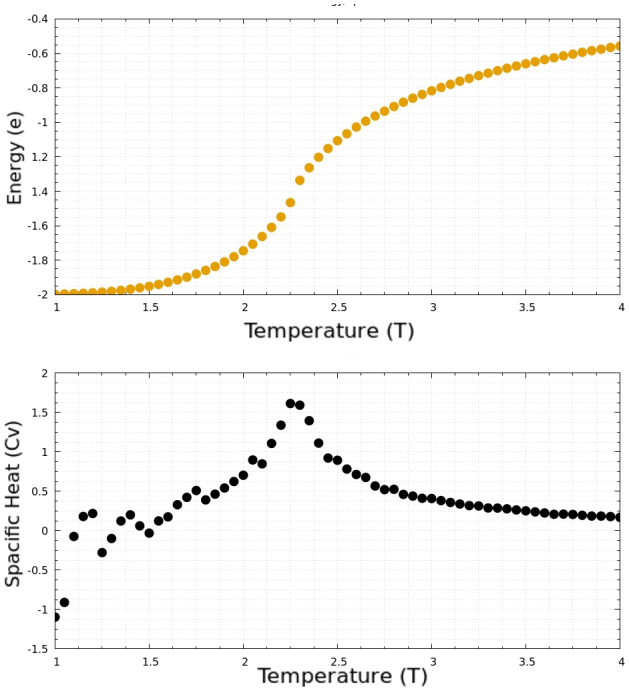


Figure 16: (a) Mean Energy (Orange points) and (b) specific heat (black points) both developing with temperature

The energy per spin for higher temperatures is relatively high which is in keeping with our expectation of having a random configuration while it stabilizes to a $E/N = 2J = 2$ at low temperatures. This indicates that the spins are all aligned in parallel.

Also for specific heat which is:

$$c_\nu = \frac{\partial H}{\partial T} \tag{8}$$

where H is the Energy and T is the temperature, at the critical temperature the specific heat tends to infinity which is a saddle point of energy curve. In figure 16(b) the specific heat per spin is a function

of temperature. We concluded that a divergence occurs at a phase transition.

The the specific heat capacity per spin that is produced in our data is not exactly the theoretical specific heat c_ν, and we will be distinguished as c'_ν. The equivalent to the theoretical value is.

$$c'_\nu = \beta^2 N(\langle e^2 \rangle) - \langle e \rangle^2) \tag{9}$$

3 Conclusion

The numerical results produced by the Monte Carlo simulation compare favourably with the theoretical results and are a valuable and efficient alternative to an exact calculation. The requirements for producing accurate results are to consider a large number of Monte Carlo steps and the accuracy is very compelling. the implemented program is well prepared to deal with different temperatures and different lattice size, so as future investigation the behaviour of Monte Carlo with different lattice size. The softwere code is avilable on github

References

[1] Nina Kuklisova,Solving the 2D Ising Model,PHYS 35200,March 2013.

[2] Jacques Kotze,Introduction to Monte Carlo methods for an Ising Model of a Ferromagnet,March 2008.

[3] Alexey Khorev,A Monte Carlo Implementation of the Ising Model in Python, August 2017.