TABLE of CONTENTS

1) INTRODUCTION

The Ising Model is named after Ernst Ising. This form of modeling is mainly used in modeling ferromagnetism in statistical mechanics, among other areas. In physics, statistical mechanics is a mathematical framework that applies statistical methods and probability theory to large assemblies of microscopic entities. It does not assume or postulate any natural laws, but explains the macroscopic behavior of nature from the behavior of such ensembles. It mainly focuses on the momentarily motions of the matters rather than time dependent behaviors.

The Ising Model consists of discrete variables representing the magnetic dipole moments of atomic spins (fig.1). Atomic spins can have one of two different states (+1 or -1), +1 means up and -1 means down. These spins are arranged in a graph, usually a lattice (fig.2), each of which can interact with its neighbors. The reason lattice is mainly used is that the local structure repeats periodically in all directions.

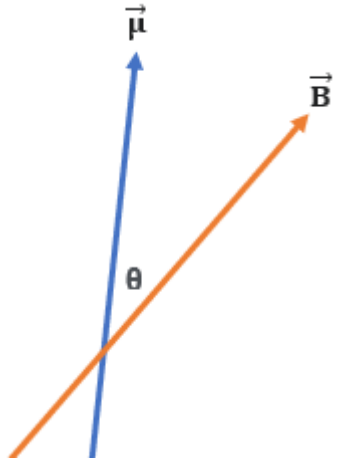


Figure.1: the magnetic dipole moments of atomic spins

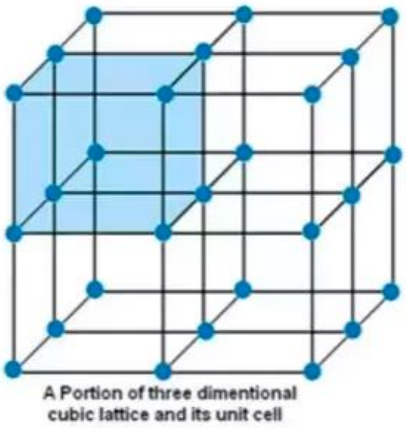


Figure.2: A simple representation of lattice that allows the atoms interact with their neighbors.

Energy→ $\mathbf{U} = -\vec{\mu} \bullet \vec{B}$

where;
μ is the spin magnetic dipole moment.
B is the magnetic field.

The interaction of neighboring spins with a lower energy causes the system to steer towards the lowest energy level, ignoring those interacting so that they can have higher energy. However, heat negatively affects this orientation by creating the possibility of forming different structural phases. As a simplifed model of reality, this model allows the identification of phase transitions. One of the most common display forms of phase transition is the 2D square-lattice Ising Model (fig.3). Altough there are different methods related to quantum field theory, the two dimensional square lattice Ising Model is usally solved using a transfer matrix model.

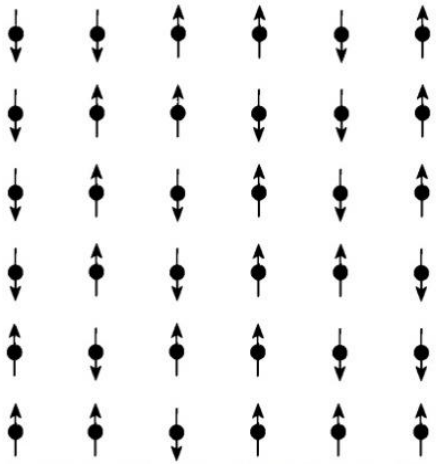


Figure.3: 2D square lattice Ising Model.

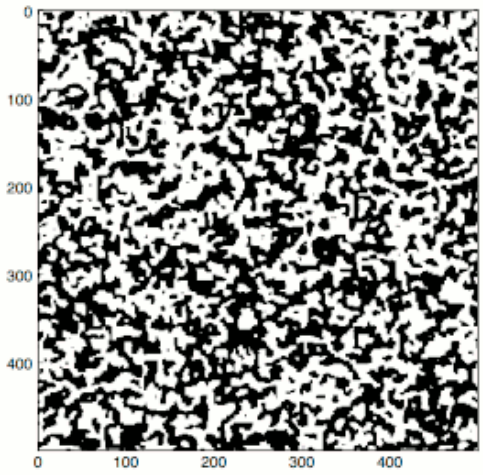


Figure.4: Quench of an Ising system on a two-dimensional square lattice

2) METHODS-DISCUSSION

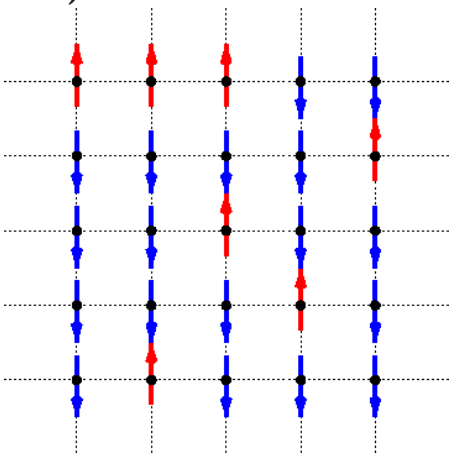
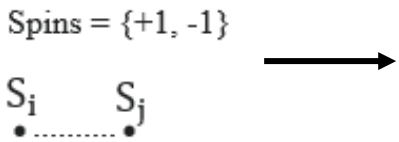


Figure.5: Two-dimensional square lattice Ising Model.

The arrows are representing the spins. The red arrows are +1(up) and the blue arrows are -1(down). The neigbors with same spin support each other but the neighbors with opposite spins behave non-supporting. To minimize the energy, all arrows should be in the same direction.



S_i comes from the i^{th} spin
S_j comes from the j^{th} spin

$$\mathbf{U} = -\mathbf{J}\mathbf{S_i}\mathbf{S_j}$$

where U is the internal energy
J is strength of magnetic interaction between spins and determined by:
$J > 0$, ferromagnetic interaction
$J < 0$, antiferromagnetic interaction
$J = 0$, the spins are noninteracting

At 0 Kelvin (absolute zero), the only thing should be cared about internal energy is the energy coming from the interaction. Total internal energy(U) becomes:

$$\mathbf{U} = \sum_{\mathbf{i,j \in nn}} -\mathbf{J}\mathbf{S_i}\mathbf{S_j}$$, where nn stands for "the nearest neighbor"

This means at 0K, all internal energy comes from interaction.
Eventually, all arrows will be in the same direction since at $T = 0K$, internal energy is in the the minumum level.

If the system has a finite temperature:

$\mathbf{Energy = H - TS}$, this energy is called Gibbs Free Energy

and $\mathbf{H = U + pv}$

where H is the enthalpy, T is the absolute temperature S is the entropy,
U is the internal energy, p is the pressure and v is the volume.

If we assume pressure and volume are negligible since we are dealing with a microsystem:

H(enthalpy) becomes U(internal energy) → $\mathbf{Gibbs\ Free\ Energy = U - TS}$

If the system is released to behave on its own, it will have zero magnetization, +1(up) numbers willl be equal to -1(down) numbers. However, the heat negatively affects this orientation by creating the possibility of forming different structural phases.

Magnetization is basically defined as the average spin of the system:
$\mathbf{M = \frac{\sum_i S_i}{N}}$, where M is magnetization and N is the number of spins.

In statistical mechanics and mathematics, a Boltzmann distribution (also called Gibbs distribution) is a probability distribution or probability measure that gives the probability that a system will be in a certain state as a function of that state's energy and the temperature of the system.

Boltzmann distribution:

$$\boldsymbol{p_k \propto e^{\frac{-E_k}{k_B T}}}$$

p_k is the probability of the system being in state k.
E_k is the energy of that state.
k_b is the Boltzmann constant.
T is the thermodynamic temperature.

$\mathbf{Z = \sum_k e^{\frac{-E_k}{k_B T}}}$, Z is defined as the summation of all configurations

Then; $\mathbf{p_k = \frac{e^{\frac{-E_k}{k_B T}}}{Z}}$

All in all, thermal average becomes:

$$\mathbf{\langle M \rangle = \sum_k p_k M_k}$$

Example to clarify:

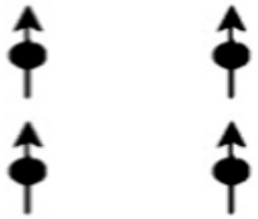


Figure.6: Schematic of an example with +1, +1, +1, +1 spins in all 4 regions

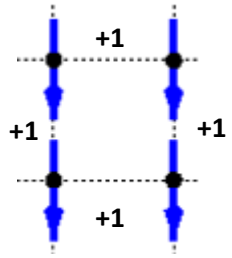
Number of all possibilities is $2^4 = 16$ since there are 4 region and each region can have the value of -1 or $+1$.
Each possibility has its own energy and because of its energy it has its own probability. In the figure on the left (fig.6), the spin values were taken as +1, +1, +1, +1, but there are 15 more different probabilities.

All the spin regions will give $-J$. Therefore, energy of the above example configuration will give $-4J$ in total.

Thus,

$$\mathbf{p_k \propto e^{\frac{-4J}{k_B T}}}$$

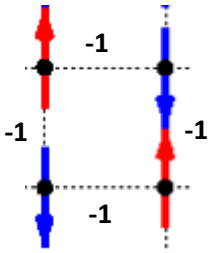
$-E_k$ was replaced with $-4J$, and k is 1 to 16 since there are 16 probabilities.



This will give 2 different arrangements, including opposite ones, resulting from

$$\binom{4}{4} * 2 = 2$$

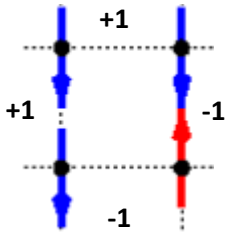
$$\mathbf{2 * e^{\frac{+4J}{k_B T}}}$$



This will give 2 different arrangements, including opposite ones, resulting from

$$\binom{4}{4} * 2 = 2$$

$$\mathbf{2 * e^{\frac{-4J}{k_B T}}}$$



This will give 12 different arrangements, including opposite ones, resulting from

$$\binom{4}{2} * 2 = 12$$

$$\mathbf{12 * e^{\frac{0}{k_B T}}}$$

As mentioned before, in this particular situation, the number of probabilities is 16(2+2+12=16).

$$\mathbf{Z = \sum_k e^{\frac{-E_k}{k_B T}} = 2 * e^{\frac{+4J}{k_B T}} + 2 * e^{\frac{-4J}{k_B T}} + 12 * e^{\frac{0}{k_B T}}}$$

Metropolis Algorithm:

The Metropolis algorithm is a method to obtain a sequence of random samples from a probability distribution from which direct sampling is difficult to obtain. This sequence can be used to compute an expected value or to calculate the distribution. When sampling from multi-dimensional distributions, the Metropolis algorithm is commonly used, particularly when the number of dimensions is large.

Without Metropolis, the solution would have 2 steps:

1) Sampling randomly:

In the spin arrangements there might be hundreds and thousands spins that would be difficult to deal with. Thanks to Metropolis Algortihm, the spins are randomly sampling and calculated seperately. Each sample will have its own energy and magnetization. At the end of the process, Summing all the samples will give the desired result.

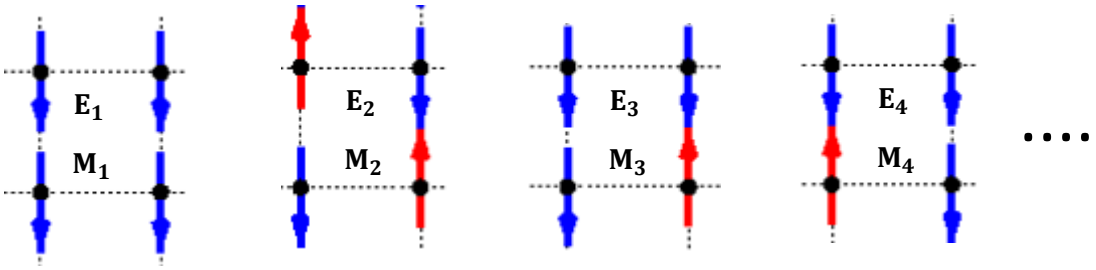


Figure.7: Different samples derived randomly from the large spin arrangement,
E is the energy of the sample. M is the magnetization of the sample.

2) Applying with the Boltzmann Distribution:

Each sample has its own probability to occur and each has its own energy along with its own magnetization. This is where Boltzmann Distribution comes in.

$$\langle \mathbf{M} \rangle = \sum_{\mathbf{k}} \mathbf{p_k M_k}\,, \text{previously discussed}$$

$$\langle \mathbf{M} \rangle = \mathbf{e}^{\frac{-\mathbf{E_1}}{\mathbf{k_B T}}}\mathbf{M_1} + \mathbf{e}^{\frac{-\mathbf{E_2}}{\mathbf{k_B T}}}\mathbf{M_2} + \mathbf{e}^{\frac{-\mathbf{E_3}}{\mathbf{k_B T}}}\mathbf{M_3} + \mathbf{e}^{\frac{-\mathbf{E_4}}{\mathbf{k_B T}}}\mathbf{M_4} \ldots$$

This is, indeed, problematic. If there is a lot of spins at very low temperature, sampling will be basically at high entropic states. However, what contribute to magnetization are the low entropic states. Therefore, when dealing with a lot of spins, finding low entropic states will be too hard, the sampling will occur at which the system will never use(very high entropic states). In such a case, one will have to sample nearly infinite times to get a proper consensus. Therefore, this approach especially fails at very low temperatures.

What Metropolis Algorithm does is:

1) **Sampling with respect to Boltzmann Distribution:**

It directly uses the Boltzmann Distribution values for each sample.

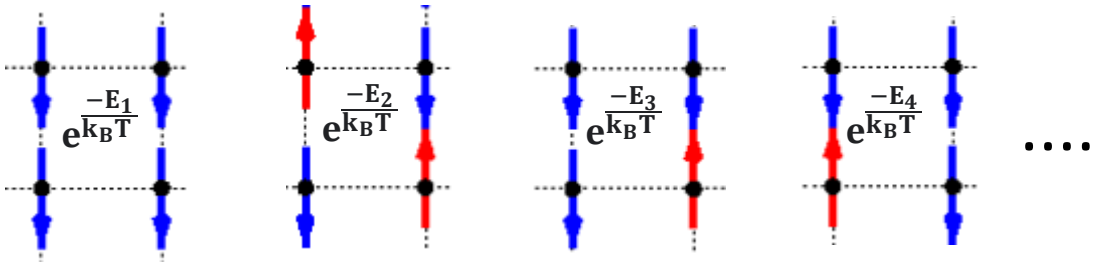


Figure.8: Different samples and their Boltzmann Distribution values

2) **Taking a normal avarage:**

This step is the same as the method without using Metropolis Algorithm. The difference between these two is that in the use of Metropolis Algorithm, the Boltzmann Distribution is applied at the beginning of the solution.

The Metropolism Algorithm has to provide relevant results, ordered states for the low temperatures and disordered states for the high temperatures.

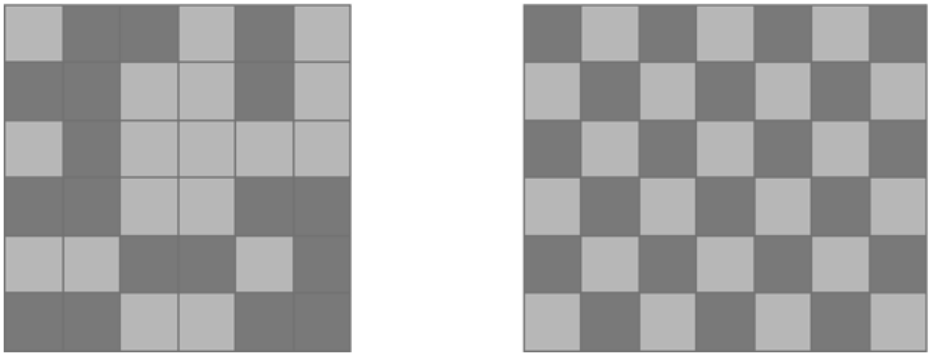


Figure.9: Representation of disordered and ordered states, the left is disordered and the right is ordered. Rise in temperature will force the state become disordered.

The Working Prenciple of Metropolis Algorithm:

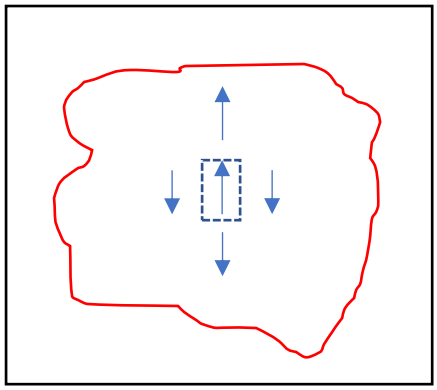


Figure.10: Spin arrangement before the middle spin is flipped

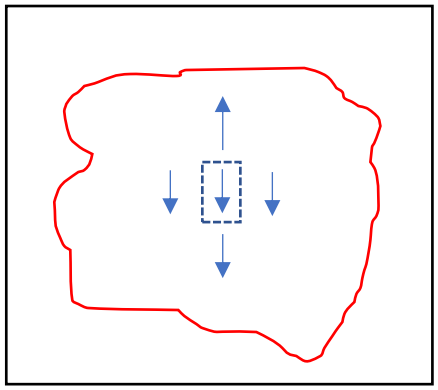


Figure.11: Spin arrangement after the middle spin is flipped

There are lots of spins out there. Among all, only one spin is chosen and investigated. Eventually the it is decided to flip the spin or leave it as it is. In the example (fig.10), if the dashed spin is flipped, the energy goes down because the spin has more down neighbors than up neighbors, so, when it is flipped, it alligns with others and that decreases the energy. This would be a favorible move. The algorithm tells to accept all favorible moves as in the example above.

- What would happen if spin were flipped in the opposite way?

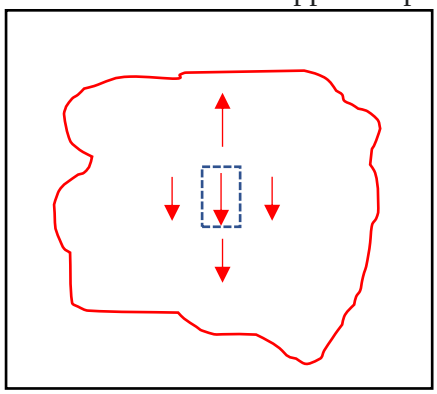


Figure.12: Spin arrangement before the middle spin is flipped

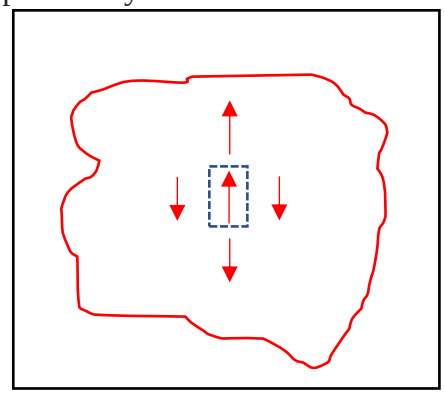


Figure.13: Spin arrangement after the middle spin is flipped

In this situation, the energy tends to increase. Actually, there is still possibility to accept this move but this would only occur under a certain probability of $\mathbf{e}^{\frac{-\Delta E}{k_B T}}$ where ΔE is the energy difference between before and after conditions. For example, if the temperature is very low, the algorithm may accept it under a very small probability, which makes sense according to probability of $\mathbf{e}^{\frac{-\Delta E}{k_B T}}$. When T is small, the probability is small too. If the temperature is 0K, then the system rejects increase in energy or any change in system. When T is 0K, the probability is 0, then the algorithm rejects to accept any change, which makes sense too. As the temperature increases, the system will have more misalignments resulting in disorderstate. This situation agrees with the statement "Rise in temperature will force the state become disordered." as stated in Figure.9.

Metropolis Algorithm can be named as differently; Metropolis-Hasting Algorithm, Monte Carlo Simulation, Monte Carlo Markov Chain, etc.

How does the flipping work?

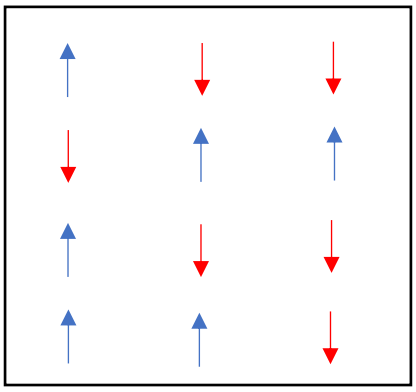


Figure.14: An example of spin arrangement

1) Monte Carlo run:

Flip attempts N times randomly, it can even be the same spin , where N is the number of spins.

To clarify the acceptance probability of flipping a spin, it is beneficial to investigate some examples:

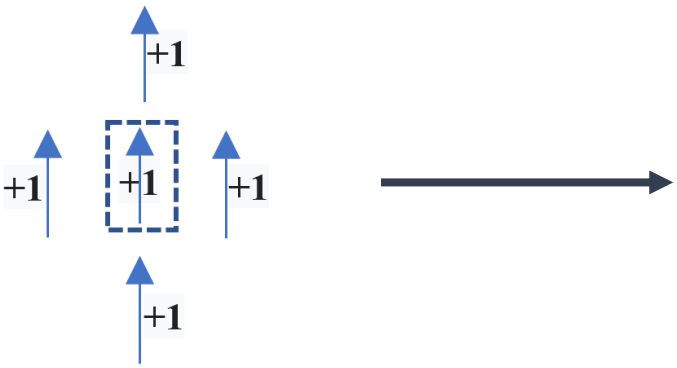


Figure.15: An example of 4-spin arrangement

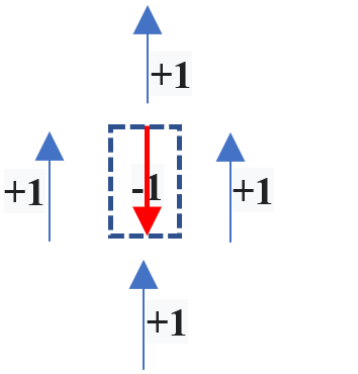


Figure.16: The same example as fig.15 but with middle spin is flipped

In the example above, the middle spin is flipped while the others stay constant. This move occurs under some probability as discussed before. To calculate this probability, one needs to examine both before and after arrangements. In the before arrangement, the sum of surrounding spins is +4 and the value of the middle spin is +1. The multiplication of these makes +4 * +1 = +4. In the after arrangement, the sum of surrounding spins is +4 since they stay constant while the middle one is spinned, and the new value of it is -1. The multiplication of these makes +4 * -1 = -4. The difference is -8. Therefore, the flipping occurs under the probability of:

$$e^{\frac{-8J}{k_B T}}$$

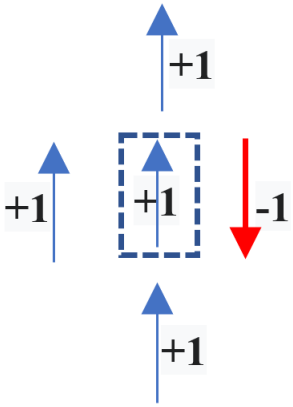


Figure.17: Another example of 4-spin arrangement

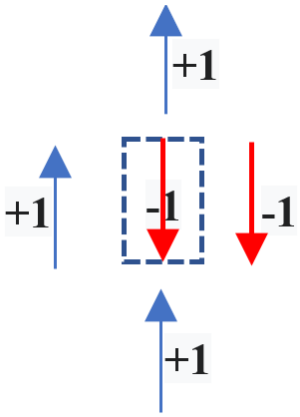


Figure.18: The same example as fig.17 but with middle spin is flipped

In the example above, the middle spin is flipped while the others stay constant. This move occurs under some probability as discussed before. To calculate this probability, one needs to examine both before and after arrangements. In the before arrangement, the sum of surrounding spins is +2 and the value of the middle spin is +1. The multiplication of these makes +2 * +1 = +2. In the after arrangement, the sum of surrounding spins is +2 since they stay constant while the middle one is spinned, and the new value of it is -1. The multiplication of these makes +2 * -1 = -2. The difference is -4. Therefore, the flipping occurs under the probability of:

$$e^{\frac{-4J}{k_B T}}$$

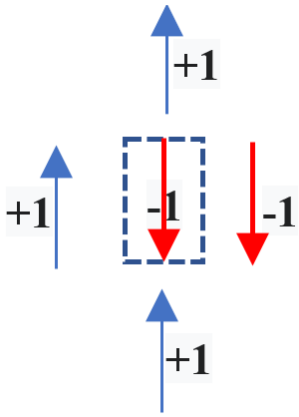


Figure.19: Another example of 4-spin arrangement

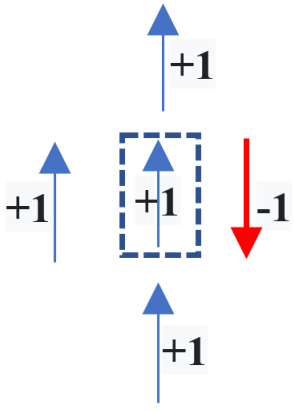


Figure.20: The same example as fig.19 but with middle spin is flipped

In the example above, the middle spin is flipped while the others stay constant. In the before arrangement, the sum of surrounding spins is +2 and the value of the middle spin is -1. The multiplication of these makes +2 * -1 = -2. In the after arrangement, the sum of surrounding spins is +2 since they stay constant while the middle one is spinned, and the new value of it is +1. The multiplication of these makes +2 * +1 = +2. The difference is +4. However, in this situation, since the energy decreases, the algorithm will accept it fully. Therefore, the flipping occurs under the probability of:

1

To generalize the acceptance probability, one can use the middle spin and sum of surrounding spins of arrangement before the change. The multiplication is represented as sum × middle. The results can be summarized in a table.

sum × middle	-4	-2	0	+2	+4
acceptance probability	1	1	1	$e^{\frac{-4J}{k_B T}}$	$e^{\frac{-8J}{k_B T}}$

Table.1: Acceptance probability distribution related to multiplication of the middle spin and sum of surrounding spins of arrangement before the change

This values can be gathered in matrix:

$$\begin{bmatrix} 1 & 1 & 1 & e^{\frac{-4J}{k_B T}} & e^{\frac{-8J}{k_B T}} \end{bmatrix}$$

Effect of temperature increase in magnetization:

As previously discussed, the change in the temperature has an effect on magnetization. The increase in temperature will negatively affect the absolute magnetization and therefore the state orderness. For example, if one decreases the absolute magnetization in a field, the particles tend to have no effect on each other and that is directly proportional to state orderness. If temperature increases, both magnetization and state orderness will decrease. At a certain point, the absolute magnetization becomes 0 and this is the same point the system is counted to pass to disordered state. Specifically this point is called critical temperature. At the critical point, there is no analytical continuity, the plot changes sharply.

$$T_c = \frac{2}{\ln(1+\sqrt{2})} \approx 2.26$$

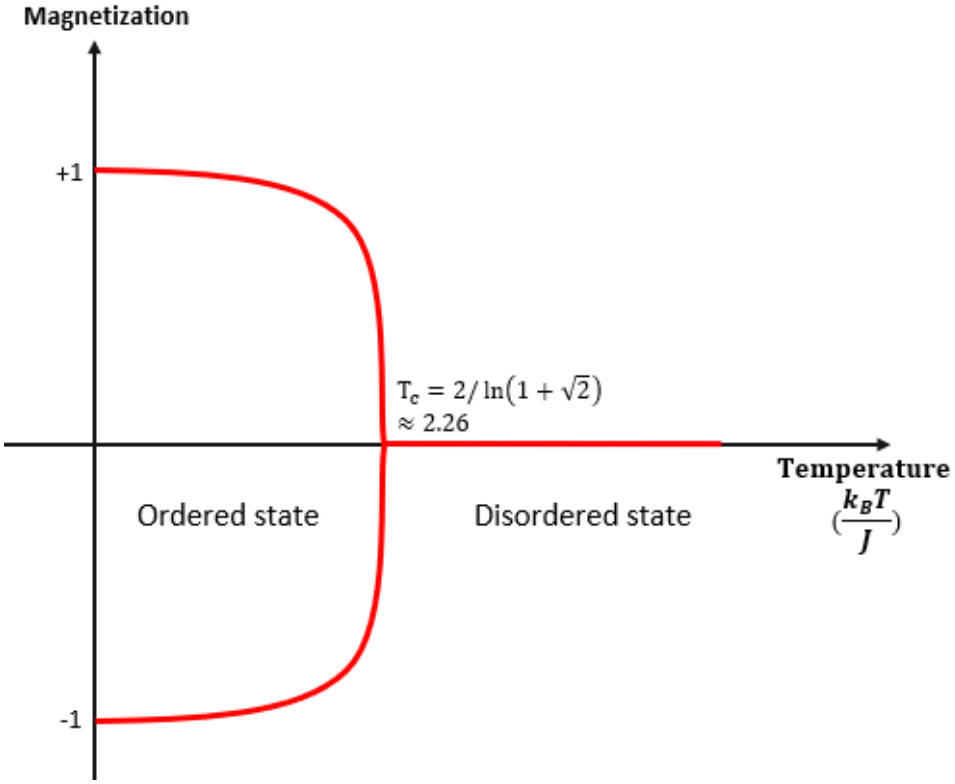


Figure.21: The effect of temperature change in magnetization and state orderness

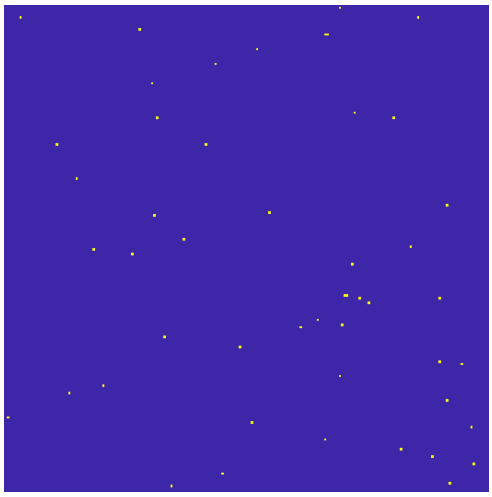


Figure.22: Initial look of the system: it mainly consists of one phase of one spin with small so small parts of the other phase in it.

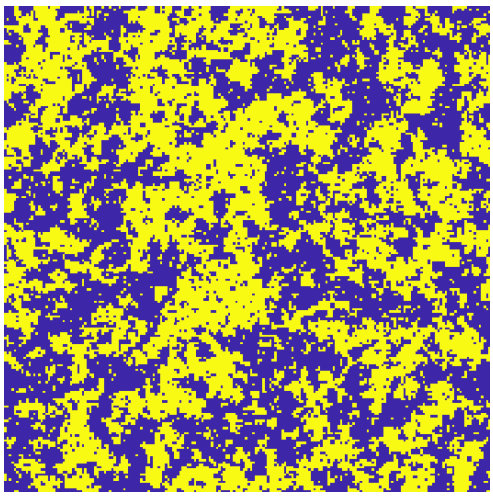


Figure.23: The look of the system after a while: the system gains clusters of the other phase in addition to smalling first large phase.

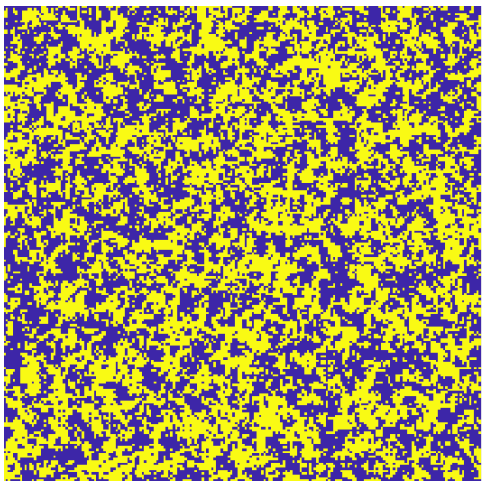


Figure.24: The look of the final version of the system: clusters diminish and leave their places to much smaller parts of the both phases.

At the beginning, the system has mainly and largly consists of one type of spin and its large cluster, as shown with blue, with time it creates second cluster, as shown with yellow. Then, the system gains little and partial arrangments of both blue and yellow. This can be clarified thinking of melting iron. At the beginning, there is a large amaount of iron. When it begins to melt some parts of the iron becomes liquid. With a relatively long time, the iron-liquid mixture is seen like iron and liquid creates a solution as seen in the third figure. The system has ordered state at the beginning but it has disordered state at the end due to the temperature increase.

3) SOLUTION

With antiferromagnetic interaction between spins, every neighboring spin wants to be the opposite to its neighbors. Therefore, minimum energy is reached when the arrangement below is satisfied:

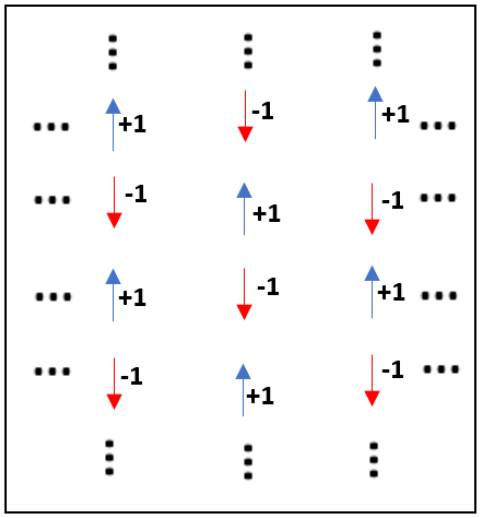


Figure.25: The desired arrangement of the spins to minimize the energy when the interaction between them is antiferromagnetic

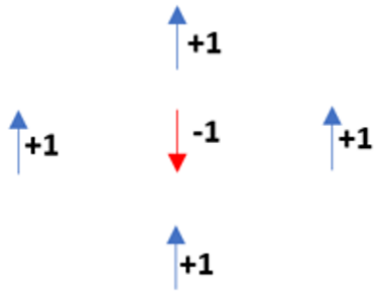


Figure.26: A part of the arrangement in fig.25

Using the formula examined before:

$\mathbf{U} = \sum_{\mathbf{i,j \in nn}} -\mathbf{JS_iS_j}$, where J is -1(antiferromagnetic)

The total energy of the partial spin arrangement on the left is:

U = -J((-1)(+1)+(-1)(+1)+(-1)(+1)+(-1)(+1))

= -(-1)(-4) = -4

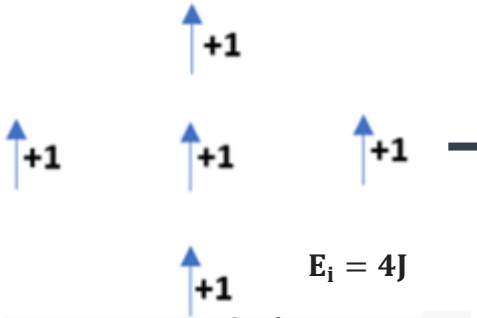


Figure.27: An example of spin arrangement

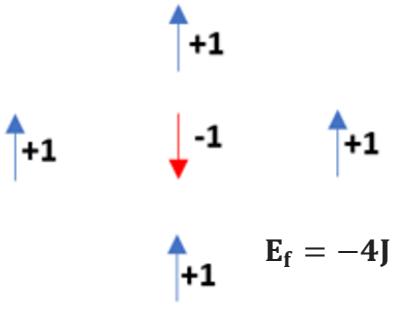


Figure.28: The same example as the fig.27 but with central spin is flipped

If the central spin is flipped the, difference of the energy ΔE will be -8J and it is accepted by the algorithm because the energy is diminished. Since it is accepted, the system will get more and more anti-parallel within the neighbors.

What if the magnetic field is included?

$\vec{\mathbf{B}}$ **,** magnetic field

When the spin is flipped, whether the energy will increase or decrease depends on the ratio of **J** and **B**.

An example to clarify:

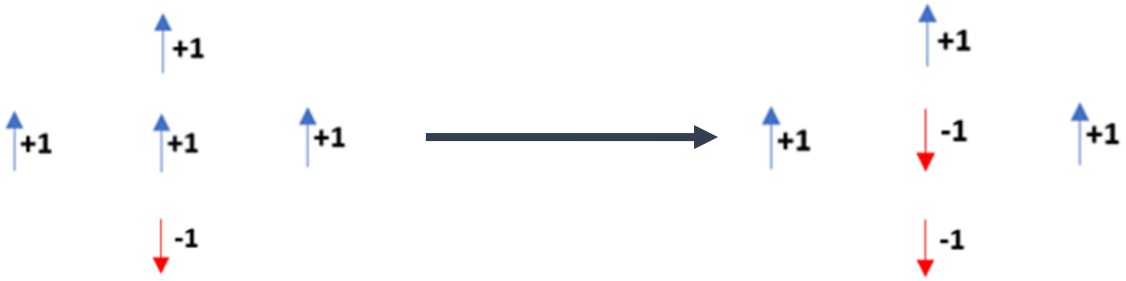


Figure.29: An example of spin arrangement

Figure.30: The same example as the fig.29 but with central spin is flipped

$E_i = -B + 2J$

$E_f = +B - 2J$

$\Delta E = E_f - E_i = 2B - 4J$

If $\Delta E > 0$, it accepts with probability of 1(fully accept)

If $\Delta E < 0$, it accepts with probability of $\mathbf{e^{\frac{-\Delta E}{k_B T}}}$

Then the acceptance probability that a spin can have to spin is $\min\left[1, e^{\frac{-\Delta E}{k_B T}}\right]$.

In the solution **antiferromagnetic** interaction between neighboring spins under the influence of an **external magnetic field is investigated by using Ising Model. The total energy of the system is given as:**

$$E = -J\sum_{nn} S_i S_j - B\sum_{all} S_i, \quad \text{nn stands for "the nearest neighbor"}$$

Dealing with antiferromagnetic interaction means J is less than 0, it is negative, as discussed before. In this particular case, J was taken -1. Here, in addition to previous discussed material, there is affect of external magnetic field. The magnetic field was taken upward and various magnitudes of 0, 0.1, 0.5 and 1.5. The dependence of temperature on the total energy of the system and magnetization is also investigated.

Previously mentioned that:
Magnetization is basically defined as the average spin of the system:
$\mathbf{M} = \frac{\sum_i \mathbf{S_i}}{\mathbf{N}}$, where M is magnetization and N is the number of spins.

4) RESULTS:

Using Magnetic Field(B) = 0:

The behaviour of the system is investigated so that its k_bT value is between 1.5 and 3. From the minumum value to maximum value, the k_bT value is increased 0.001 at each step. At each temperature, the spins are examined 100000 times.

200 x 200 square is used, which means there are 40000 spins in the square lattice. Magnetization and the total energy are calculated for each temperature and the dependence of temperature on magnetization and total energy is examined.

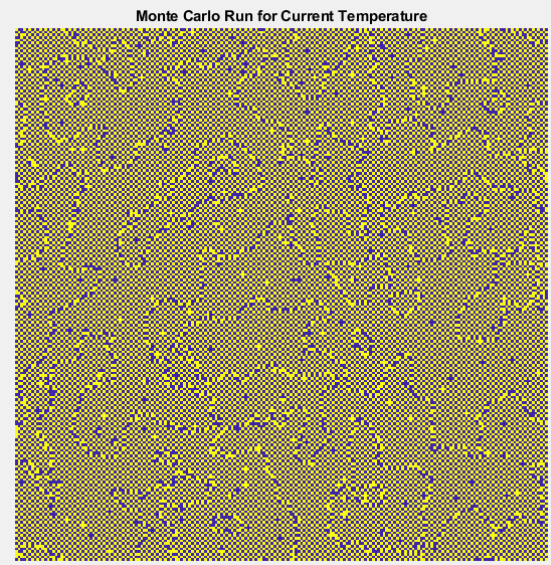


Figure.31: Antiferromagnetic interaction of the first experiment with low temperature

k_bT is 1.507

Total energy = -112954

Magnetization = 0.0038

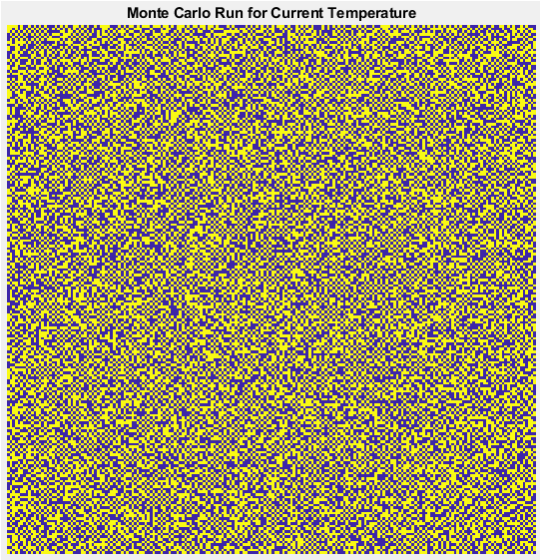


Figure.32: Antiferromagnetic interaction of the first experiment with high temperature

k_bT is 3.000

Total energy = -65504

Magnetization = 0.0037

Initially, the appearance of the lattice is like a chessboard with small disorderness. If the initial temperature was taken lower than the given, it would be even more ordered. After increasing the temperature, the state gets disordered. Since the interaction is antiferromagnetic and specifically J is -1, the spins are in the opposite direction with the neighbor spins. The total energy after increasing temperature increases and it is expected because to increase the temperature, there should be additional external heat applied, the more energy given, the higher total energy. In addition, even if the magnetization changes during the increasing the temperature, the change is not that high.

Using Magnetic Field(B) = 0.1:

The behaviour of the system is investigated so that its k_bT value is between 1.5 and 3. From the minumum value to maximum value, the k_bT value is increased 0.001 at each step. At each temperature, the spins are examined 100000 times.

200 x 200 square is used, which means there are 40000 spins in the square lattice. Magnetization and the total energy are calculated for each temperature and the dependence of temperature on magnetization and total energy is examined.

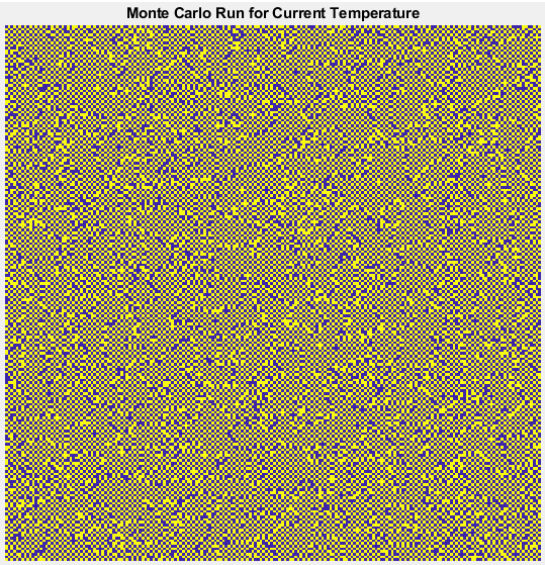


Figure.33: Antiferromagnetic interaction of the second experiment with low temperature

k_bT is 1.509

Total energy = -119360

Magnetization = -0.0092

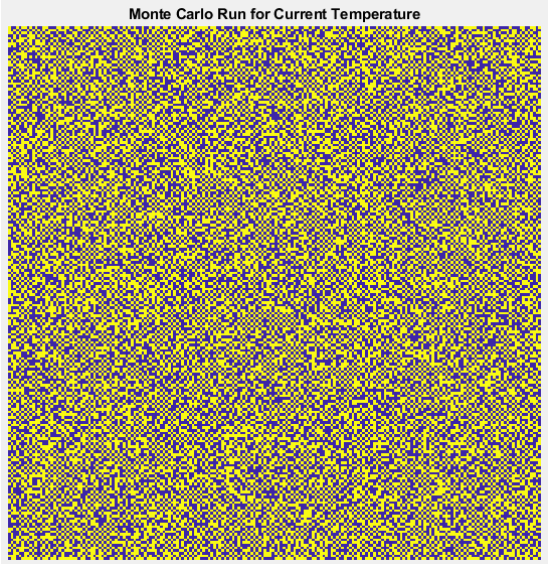


Figure.34: Antiferromagnetic interaction of the second experiment with high temperature

k_bT is 2.990

Total energy = -68679

Magnetization = -0.0023

The lattice initially has the appearance of a chessboard with slight disorder. It would be much more ordered if the initial temperature was lower than the given. The state becomes disordered as the temperature rises. The spins are in the opposite direction with the neighbor spins since the interaction is antiferromagnetic and J is -1. The total energy increases as the temperature rises, which is to be expected because to raise the temperature, more external heat must be applied; the more energy provided, the higher the total energy. During the process of increasing temperature, magnetization increases or decreases step to step but in general, one can say the magnetization of the interaction of spins of the system increases as the temperature increases.

Using Magnetic Field(B) = 0.5:

The behaviour of the system is investigated so that its k_bT value is between 1.5 and 3. From the minumum value to maximum value, the k_bT value is increased 0.001 at each step. At each temperature, the spins are examined 100000 times.

200 x 200 square is used, which means there are 40000 spins in the square lattice. Magnetization and the total energy are calculated for each temperature and the dependence of temperature on magnetization and total energy is examined.

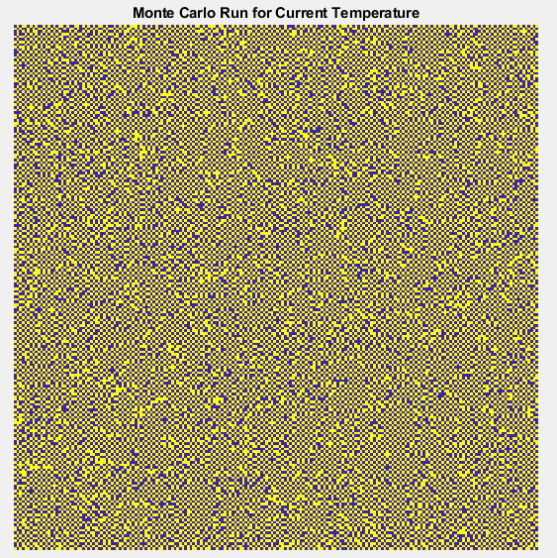


Figure.35: Antiferromagnetic interaction of the third experiment with low temperature

k_bT is 1.5010

Total energy = -124419

Magnetization = 0.0066

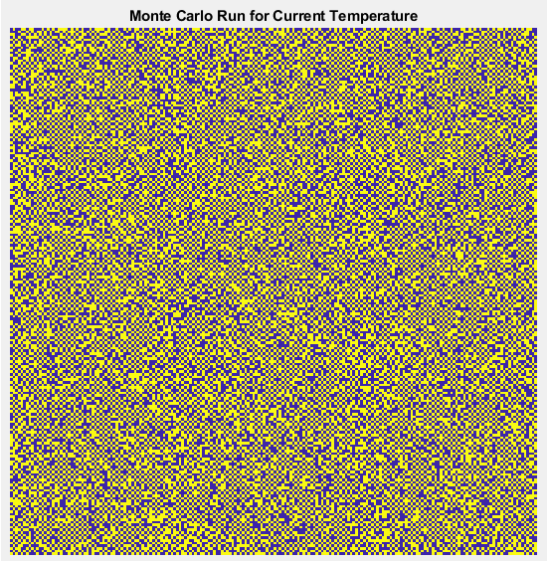


Figure.36: Antiferromagnetic interaction of the third experiment with high temperature

k_bT is 2.990

Total energy = -86895

Magnetization = 0.0095

The lattice initially has the appearance of a chessboard with small disorder. It would be much more ordered if the initial temperature was lower than the given. If the temperature increases, the state becomes more disordered. Since the interaction is antiferromagnetic and J is -1, the spins are in opposition to their neighbors' spins. When the temperature rises, the overall energy increases, which is to be expected because more additional heat must be added to largen the temperature; the more energy produced, the higher the total energy. During the process of increasing temperature, magnetization generally increases.

Using Magnetic Field(B) =1.5:

The behaviour of the system is investigated so that its k_bT value is between 1.5 and 3. From the minumum value to maximum value, the k_bT value is increased 0.001 at each step. At each temperature, the spins are examined 100000 times.

200 x 200 square is used, which means there are 40000 spins in the square lattice. Magnetization and the total energy are calculated for each temperature and the dependence of temperature on magnetization and total energy is examined.

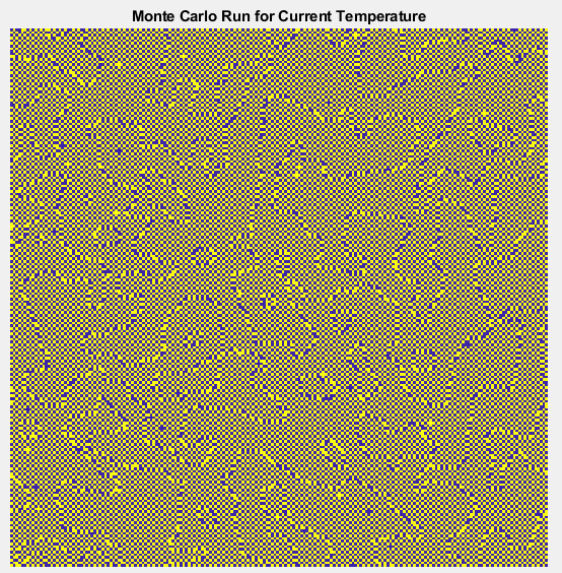


Figure.37: Antiferromagnetic interaction of the fourth experiment with low temperature

k_bT is 1.5040

Total energy = -154499

Magnetization = -0.0037

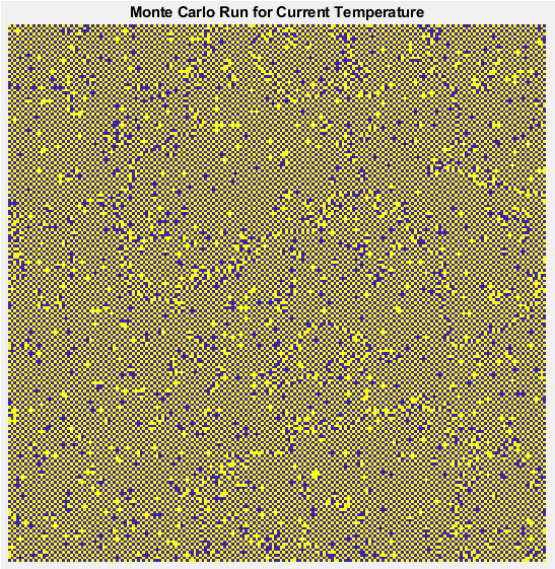


Figure.38: Antiferromagnetic interaction of the fourth experiment with low temperature

k_bT is 3.000

Total energy = -134544

Magnetization = -0.0030

The lattice initially has the appearance of a chessboard with small disorder. If the temperature increases, the state becomes more disordered. Since the interaction is antiferromagnetic and J is -1, the spins are in opposition to their neighbors' spins. When the temperature rises, the overall energy increases, which is to be expected because more additional heat must be added to largen the temperature; the more energy produced, the higher the total energy. However, in this particular situation, the change in total energy is not much. This may be resulted from the large effect of magnetic field. Besides, the magnetization changes slightly.

5) CONCLUSION

The Ising Model consists of discrete variables representing the magnetic dipole moments of atomic spins. Atomic spins can have one of two different states (+1 or -1), +1 means up and -1 means down. The interaction of neighboring spins with a lower energy causes the system to steer towards the lowest energy level, ignoring those interacting so that they can have higher energy. In materials that exhibit antiferromagnetism, the magnetic moments of atoms or molecules, usually related to the spins of electrons, align in a regular pattern with neighboring spins (on different sublattices) pointing in opposite directions.

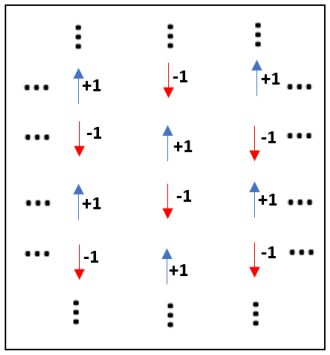
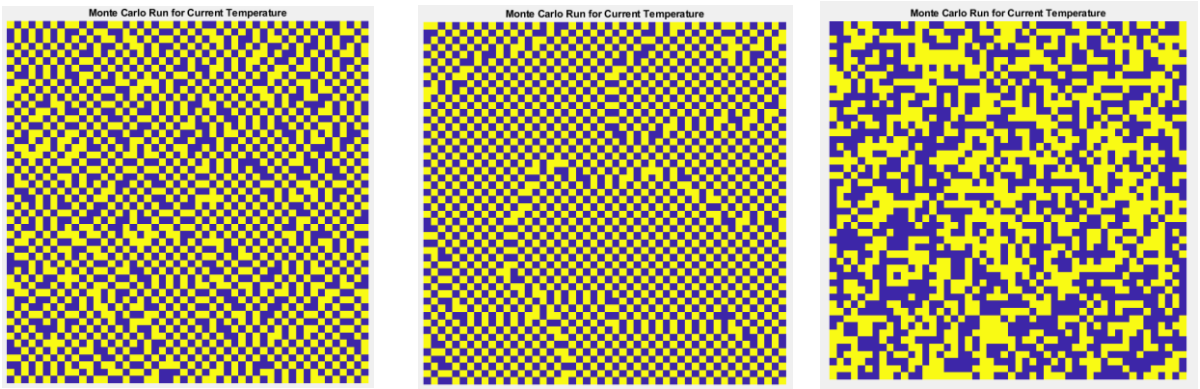


Figure.39: Arrangement of antiferromagnetic interaction of spins.

As the magnitude of the magnetic field increases, the effect of temperature on the energy of the system decreases because the magnetic field uses its own physics contrary to the changes in the system. Again, for this reason, the magnetism in the system is not affected much by the temperature because the magnetism in the system is more affected by the applied magnetic field compared to the increasing temperature.

The increase in temperature causes the arrengement to become scattered, uneven, and disordered. The initially regular spin arrangement becomes disordered as its temperature rises. While temperature has a direct relationship with total energy, it does not directly affect magnetization as clarified.

When the system is heated, the arrangement tends to be ordered for a short period of time. However, as mentioned before, after the critical temperature it starts to become disordered and any increase in temperature disrupts the orderness of the system. This situation is stated below using a 50 x 50 square lattice.



k_bT is 1.5010 k_bT is 1.5940 k_bT is 5.4230

Figure.40: An example of antiferromagnetic interaction at different temperatures

6) CODE REVIEW

```
clear
N = 200; Q = 100000; K = 100; J = -1; kbT = 1.5;
Tmin = 1.5; Tmax = 3; dT = 0.001;
a = ceil(rand(N,N)*2)*2 - 3;
B = 0; % 0, 0.1, 0.5, 1.5
```

Square lattice determination, review determination for each spin (Q),
Minimum and maxiumum values of k_bT,
Determination of initial spins

```
for q = 1 : Q
    kbT = kbT + dT;
    if (kbT < Tmin) || (kbT > Tmax)
        dT = -dT;
    end
    kbT;
```

Letting temperature to increase with step size 0.001

```


    r0 = ceil(rand(N^2,2)*N); rn = mod(r0 - 2,N) + 1; rp = mod(r0,N) + 1;
    r = rand(N^2,1);

    total_energy = 0;
    spin_total = 0;
```

Finding coordinates of the the spins,
Describing the initial values of total energy and total spin(to calculate magnetization later on)

```
    for n = 1 : N^2
        m = (a(rn(n,1),r0(n,2)) + a(rp(n,1),r0(n,2)) + ...
             a(r0(n,1),rn(n,2)) + a(r0(n,1),rp(n,2)))... % sum of outer shell
            *a(r0(n,1),r0(n,2)); % multiply with center divide by 2 add 3

        dE= 2*B-2*m;
        if r(n) < exp(-dE/kbT)
            a(r0(n,1),r0(n,2)) = -a(r0(n,1),r0(n,2)); % flip the spin
        end
        total_energy = total_energy + -J*((a(rn(n,1),r0(n,2)) + a(rp(n,1),r0(n,2)) + ...
             a(r0(n,1),rn(n,2)) + a(r0(n,1),rp(n,2)))... % sum of outer shell
            *a(r0(n,1),r0(n,2))) - B*a(r0(n,1),r0(n,2));
        spin_total = spin_total + a(r0(n,1),r0(n,2));
    end
```

Multiplying central spin with sum of its neighboring spins,
Describing change in energy and using it to determine acceptance probability,
Taking new temperature and magnetic field into account , describing new total energy and total spin

```
    magnetization = spin_total/N^2;
    disp("kbT total energy and magnetization")
    kbT
    total_energy
    magnetization
```

Calculating magnetization,
Showing k_bT, total energy and magnetization

```


    imagesc(a);
    title(['Monte Carlo Run for Current Temperature']);
    axis equal off;
    drawnow;
end
```

Creating 2D square lattice graph