STUDY OF THE ISING MODEL

2009
Project SEED
Research

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ABSTRACT

For nine weeks research was conducted, studying the whole process of the Monte Carlo Technique. Our main objective was to utilize the Monte Carlo technique to simulate mathematical systems. The processes revolved around the whole concept of the Ising Model. Studying it's theory we gained knowledge on how the whole process was conducted. With that knowledge we successfully approached our goal with astounding result. In this detailed report, I will emphasize the theory of the Ising Model, our computations and result, and how those aspects brought forth the success of the Monte Carlo Technique.

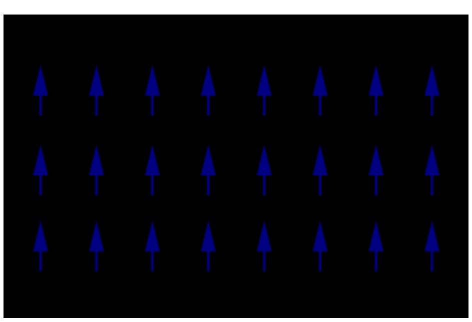
THEORY

Magnets are utilized by millions of people worldwide, but most may not realize every time they open their fridge our listen to their mp3 players is that they are using a quantum mechanical phenomenon. A specific type of magnetism I will attempt to focus on is Ferromagnetism. It is a mechanism in which electrically uncharged materials strongly attract. The following paragraphs emphasize on categories relating to ferromagnetism which include electron spin, ferromagnetic phase transition, phase transition, Curie temperature, and the physicist Ising Model.

Ferromagnetism

In Addition to this physical concept, it is a mechanism that is associated with certain (such as iron) materials that are easily magnetized in strong magnetic fields. The magnetization approaches a definite limit called saturation. When these ferromagnetic materials are heated to a certain temperature called the curie point, they lose their characteristic properties and become less magnetic. However they become ferromagnetic upon cooling.

The magnetism in the material is caused by the alignment patterns of their constituent atoms, which behave like elementary electromagnets. Ferromagnetism's concept explains that some species of atoms pose a magnetic moment-that is, that such an atom itself is an elementary electromagnet produced by an electron spin, which I will explain later on.

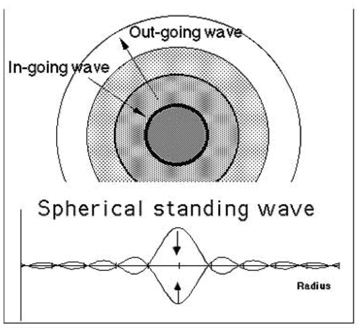


This image depicts the ferromagnetic ordering of magnets in a 2 dimensional lattice

Electron Spin

An electron sin is an intrinsic property of electrons. Electrons have intrinsic angular momentum, basically the spherical rotation of a sub-atomic particle. A highly successful mathematical theory of spin has been developed by P.A.M Dirac and others. An electron's angular momentum is characterized by a quantum number of ½. There are two types of evidence which suggest an additional property of the electron. On was the closely spaced splitting of the hydrogen spectral lines, also called fine structured. The other was the stern-Gerlach experiment in 1922. It showed that a beam of silver atoms directed through an inhomogeneous magnetic field would be forced into two beams.

The following diagram shows a cross-section of the spherical wave structure. It includes an inward and outward moving wave. Both waves combine to form a single dynamic standing wave structure. Its center is the nominal location of the electron. The waves are a part of quantum theory, not electric theory. This is due to the amplitude a quantum wave being a scalar number. The lower diagram depicts the same quantum wave amplitude plotted along a radius outwards from the electron center. The lower diagram is a portion from the upper diagram.



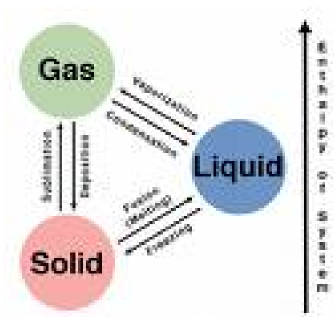
Curie temperature

Curie temperature is the temperature at which certain magnetic materials undergo a sharp change in their magnetic properties. They lose their characteristic ferromagnetic ability, as I mentioned earlier. The Curie temperature for iron is 768°C or 1414 °F. At temperatures below the Curie point the magnetic moments are partially aligned within magnetic domains. As the temperature increase towards the Curie point, the magnetization within each domain decrease. The energy of the atoms are to great for them to join together to form small magnetic areas in the material.

Phase transition

Phase transition is basically is basically a natural physical process. It takes a given medium with given properties and transforms some or that entire medium, into a new medium with new properties. For example in thermodynamics, a phase transition is the transformation of a thermodynamic system from one phase to another. At the point of transition, physical properties undergo sharp change, for instance, the boiling of liquid water result in the formation of steam.

Pertaining to ferromagnetism, a phase transition occurs between the ferromagnetic and paramagnetic phases of magnetic materials at the Curie point. When the temperature increases beyond the point, the second-order of phase transition occur, resulting in the system being unable to maintain a spontaneous magnetization. It is a second order of phase transition because it is not involved with the latent heat of the material.



Ising Model

The Ising Model, named after Ernst Ising, is a mathematical model used in statistical mechanics. When utilized in this phenomena , bits of information, interacting in pairs, produce collective effects. It comprise of a collection of variables called spins, which takes on a the value 1 or -1. The spins Si interact in pairs. Their energy has one value when the two spins comparable, and a second value when different. Because the model is statistical, the energy is the logarithm of the probability. This model was develop through the inspiration of ferromagnetism. The model basically explained whether is was possible for a large portion of electron to be forced into spinning in the same direction.

The energy of the Ising Model is defined in the following diagram

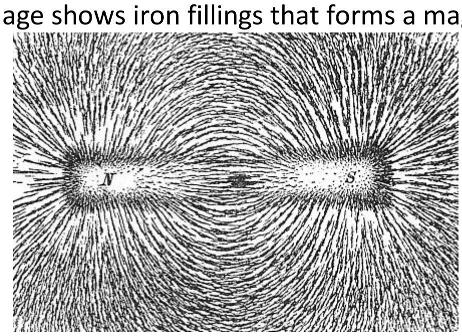
$$E = -\sum_{ij} J_{ij} S_i S_j$$

The sum counts each pair only once. The product of spins is either +1 if the two spins are aligned. If they are different the product will result in -1. J is half the difference in energy between two possibilities. Magnetic interactions usually align spins relative to one another. The spins become randomized due to the thermal energy being greater than the strength of the interaction.

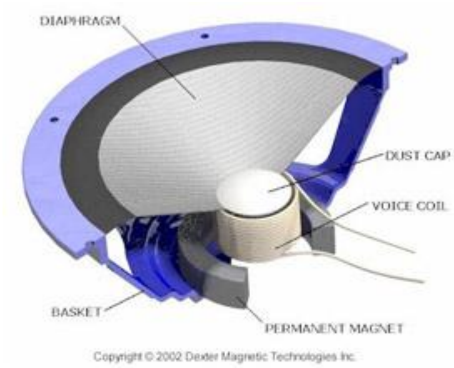
Magnets

Magnets impact the modern world in a vast influential perspective, which are both fascinating and interesting. They have incredible capabilities that attract and repel to others. Mankind have modified the capabilities of magnets and soon discovered how to synthesize these capabilities bringing forth the electromagnet. This is done by coiling wires around into a loop, electric current is passed through the coils and a magnetic field is created. When an object attract or repel a magnet, it is said that such objects have high permeability, meaning there level of magnetism. Permanent magnets are those that don't require outside influences to have a magnetic field.

This image shows iron fillings that forms a magnetic field produced by a bar magnet.



We live in a technological world that utilizes magnets 24/7. I used applications that involve magnets. For instance they have been converted into magnetic strips where information can be stored, like my flash drive. ATM cards also employ a strip of magnetic fields. The strip contains all the information necessary to access their accounts that pertains to the card. Microphones and speakers also need magnets in order to work. They use a combination of permanent magnet and an electromagnet. The speakers use the electromagnet to carry the signals that generate a varying magnetic field that influences the motion of the magnetic field that is generated by the permanent magnet. The sound is produced by the recurring force that moves the cone. Although the microphone has the same concept, it is done in a reverse manner. Television sets and computer monitors also you magnets to generate images. One application which I find amusing is refrigerator magnets.

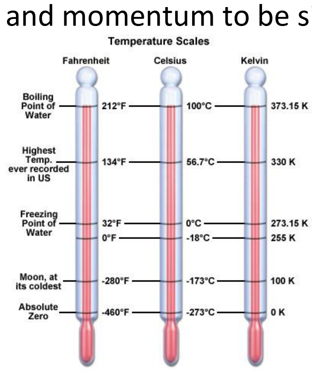


Parts of a speaker

Another interesting application I know is the maglev train. Its rail transport uses magnetic levitation. The magnetic levitation is a method by which an object is suspended using a magnetic field. The electromagnetic force is used to resist the effects of the gravitational force. Magnets impact everyday life overall. They are a vital tool need in order for most applications to work. This phenomenal tool have helped the modernized world that we currently live in.

Absolute Temperature(K):

Absolute temperature, proposed by William Kelvin, is a temperature measured from absolute zero on the Kevin scale. On the Kelvin scale the coldest temperature possible has a value of 0 kelvin, -273°C, a is called the absolute zero. Absolute zero cannot be reached by artificial or natural processes. There are several thermodynamic consequences due to having a limited temperature. For instance, absolute zero all molecular motion do not stop but does not have enough energy to transfer to other systems, leaving energy to be minimal at 0 Kelvin. In addition a partial at absolute temperature would remain at rest, resulting in both its position and momentum to be simultaneous. Theoretically it is not possible to call any substance to 0



,but scientists have achieved temperature close to absolute zero.

Energy:

In physics energy is a scalar quantity that describes the amount of work that can be performed by a force, which is an attribute of objects and systems pertaining to the conservation law. The

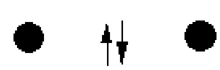
law of conservation, which is one of the most important and firmly established laws of physics basically states that energy cannot be destroyed nor created, and is the same in a closed system. Energy absorbed into a system must always equal to the energy released. The earth is considered a closed system. The Laws of physics dictates that energy can be change from one form to another. There are various forms of energy; kinetic energy, potential energy, mechanical energy, nuclear energy etc. But these forms aren't directly used in modern day applications. That's where electricity plays a role. Since
electricity is the primary form of energy consumed by the majority of the world's population, power plants converts heat from burning biomass or kinetic energy from falling water into the energy that flows through the wire in our homes.

Forms of Energy:

Kinetic energy (KE) is the energy associated with moving objects. The formula for this energy in motion is described as $KE = \left(\frac{1}{2}\right) mv^2$, where m; is the mass of an object, and v is the velocity, where m; is the mass of an object, and v is the velocity of the object. Hence this type of energy is dependent on velocity and mass. Potential energy (PE) is the energy stored in an object, or the potential of the object to do work. For example, a rock at the top of a cliff has more potential energy than one on the ground. Once the rock moves the potential energy decrease and eventually converts into kinetic energy.

Exchange Interaction:

According to physics, the exchange interaction is basically a quantum mechanical effect that increases or decreases the expectation value of the energy or distance between two or more of the same particle when their wave functions overlap. In an exchange interaction identical particles with spatially symmetric functions appear farther apart. The interaction is merely a quantum mechanical effect without any analog in classical mechanics. The exchange interaction between neighboring magnetic ions will force the individual moments into parallel ferromagnetic or anti-parallel anti-ferromagnetic alignment with their neighbors. There are three types of exchange, direct exchange, indirect exchange and super exchange. One in particular that I will discuss is direct exchange. Direct exchange occurs between moments which are close enough to have sufficient overlap of their wave functions. Take for instance two atoms with one electron each. When the atoms the close atoms spend most of their time between the nuclei there Coulomb interaction is minimal. The electrons spend most of their time in between neighboring atoms when the interatomic distance is small. The following is an anti parallel alignment for small interatomic distances.



Another figure describes the parallel alignment for large interatomic distances:

When farther apart, the atoms spend their time in this state in order to decrease the electron-electron repulsion, resulting in parallel alignment.

Boltzmann :

This constant derives its name from the Austrian physicist Ludwig Boltzmann (18844 1906). The Boltzmann constant(k) is a physical constant that defines the relation Between absolute temperature and the kinetic energy contained in each molecule of an Ideal gas. It is equal to the ratio of the gas constant ($8.314\ \ 472(15)\ \mathrm{J\ \ K^{-1}\ \ mol^{-1}}$) to the Avogadro's constant (6.022169×10^2). The following is the equation for Boltzmann constant: $k = \frac{R}{N_a}$. Boltzmann constant is a relationship between macroscopic and microscopic physics. On a Macroscopic level, the ideal gas law states that, for an ideal gas, the product of pressure p and volumes V is proportional to the product of amount substance n and absolute temperature T. Described as follows: $pV = nRT$. Where R is the gas constant ($8.314\ \ 472(15)\ \mathrm{J\ \ K^{-1}\ \ mol^{-1}}$).

2D Ising Model

The Ising Model, mentioned earlier, is a standard model that provides a simplified microscopic description of ferromagnetism. It merely explains the ferromagnetic phase transition from the paramagnetic phase at high temperatures to the ferromagnetic phase below the curie temperature Tc. The techniques and methods that have been formulated for this model were generalized and adapted similar models and problems. In following paragraphs emphasize on the two dimensional Ising model. The two dimensional Ising is normally used to model the behavior of simple magnets. It consist of a set of magnetic spins arranged on a regular square lattice. The energy of the system is determinedbut the sum of interactions between a spin and its neighbors on the lattice. The following diagram shows the equation for energy in a 2D model.

$$E = -\sum_{i=1} \quad (S_I S_I + 10 + S_I S_I + 01)$$

Where Σ is the sum of all site.
Si "site" index the spin to the bottom + Si "site index" times the spin to the right.
The following is a diagram of a 2 dimensional 3 by 4 lattice, in which it includes the periodic Boundary condition.

$$\begin{matrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ -1 & -1 & 1 \end{matrix}$$

Periodic boundary conditions are often used to simulate a large system by modeling a small part that isfar from its edge. In the two dimensional model each spin at the edge couples with the spins on theother end of its row and colomn. For example the last spin in the first row interacts the spins at the beginning of it's row and with the spin on the other end of its colomn.

Magnetization

Magnetization is very simialr to energy. It describes the state of a system in a certain configuration. The following is the formula for magnetization

$$M = \frac{1}{n}\sum Si$$

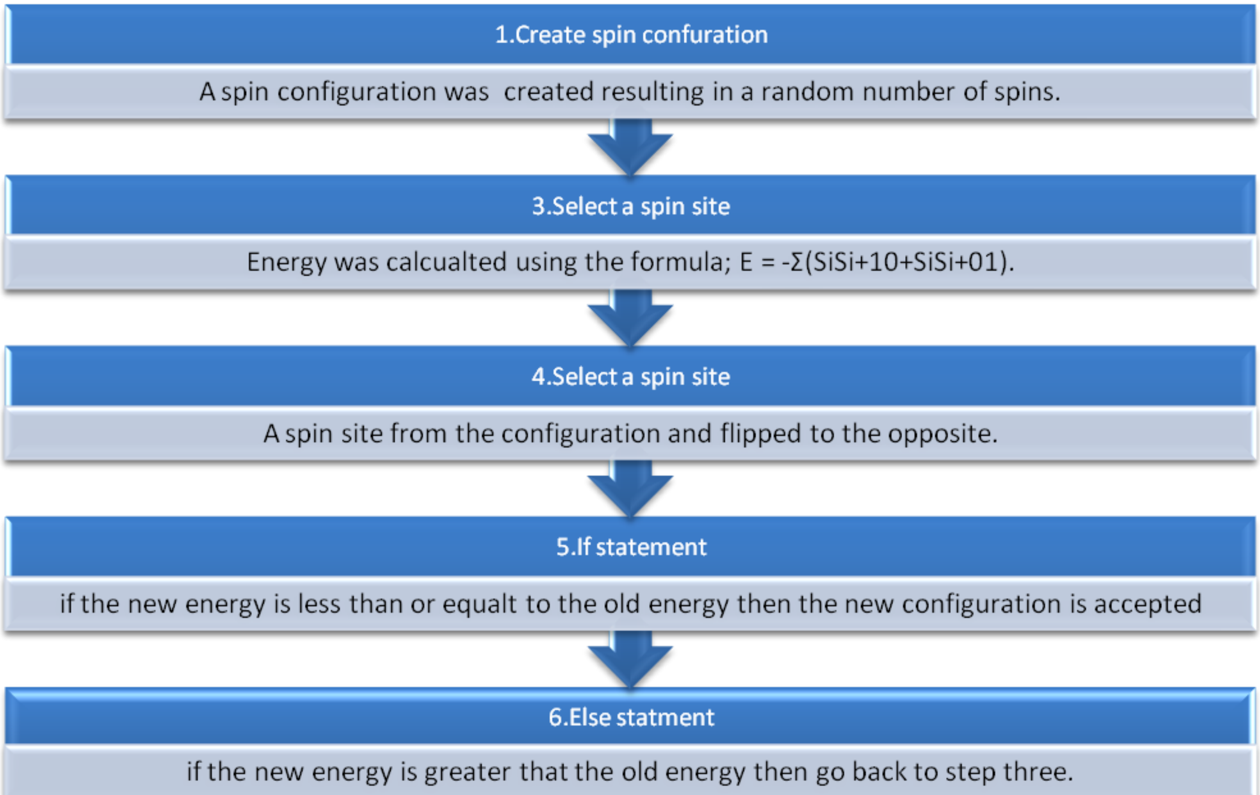
Where 1/n "total number of spins" * the site index(Si).

METHOD

Monte Carlo Technique

This is the point where temperature is introduce, with the usage of the Boltzmann and probability function. Mentioned previously, Monte Carlo is a class of computation algorithms, which rely on random numbers to compute its results. Because of its reliance on random numbers, the methods are suited calculation by a computer. Thus the method is best suited for how calculations.

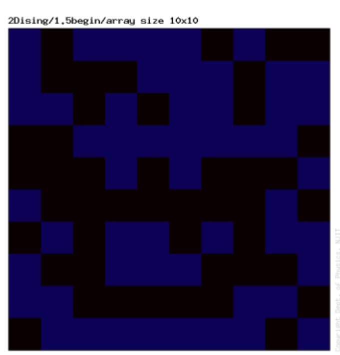
Flow Chart

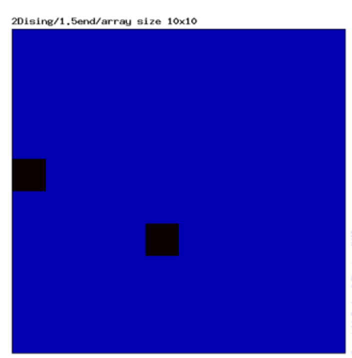


Results with various temperatures:

1.5 temp.

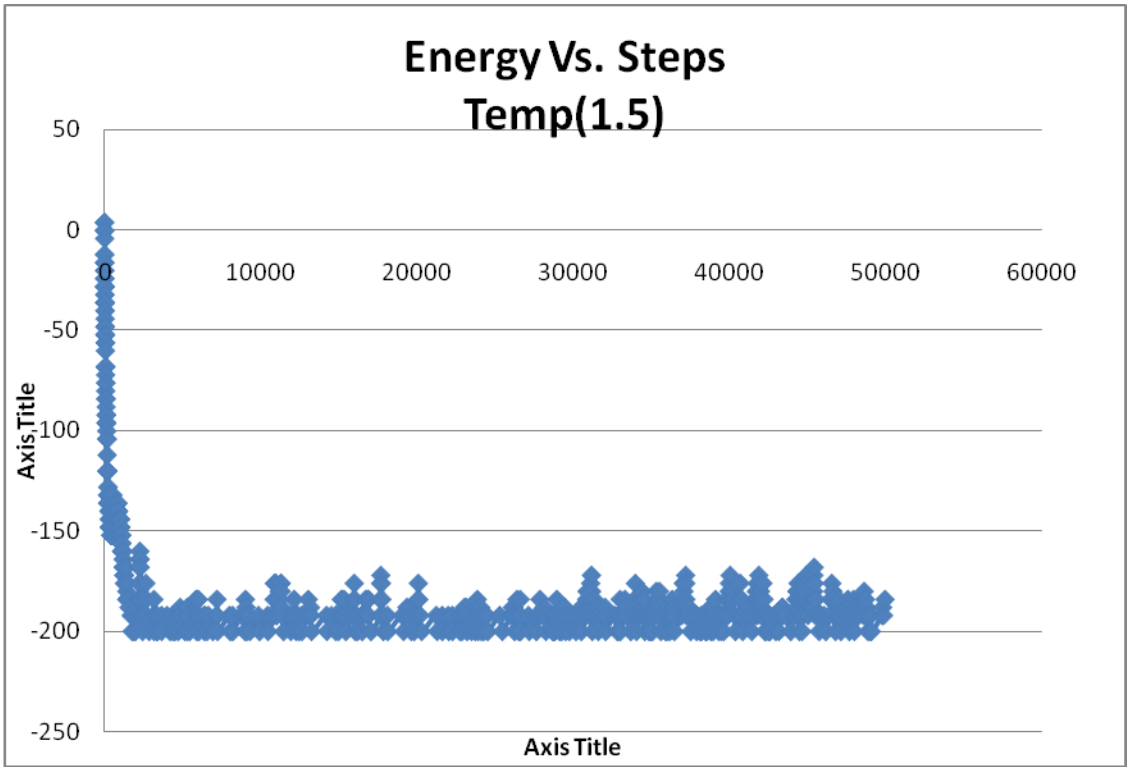
Spin map: initial final

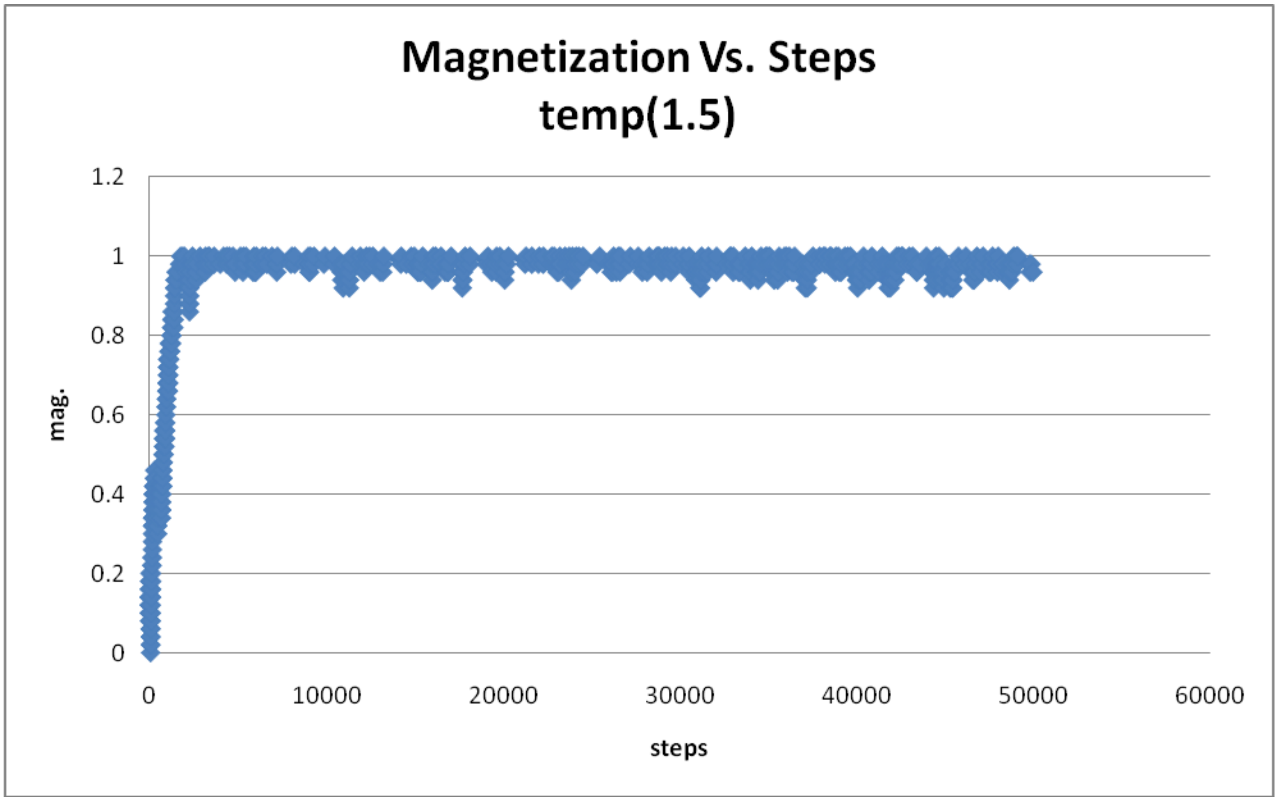




Excel Data plot:

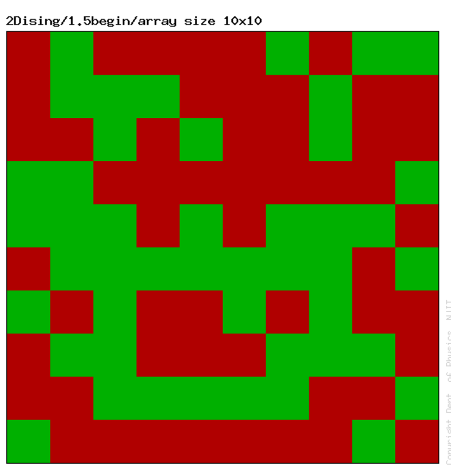
The first data plot shows a graph of a 10x10 system with fluctuating energy levels. The seconds shows the imagination levels for the 1.5 temperature. Once the energy levels are fluctuating, a better average magnetization result will occur for the tested temperature

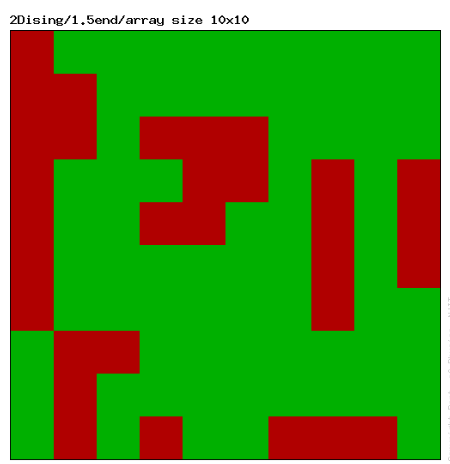




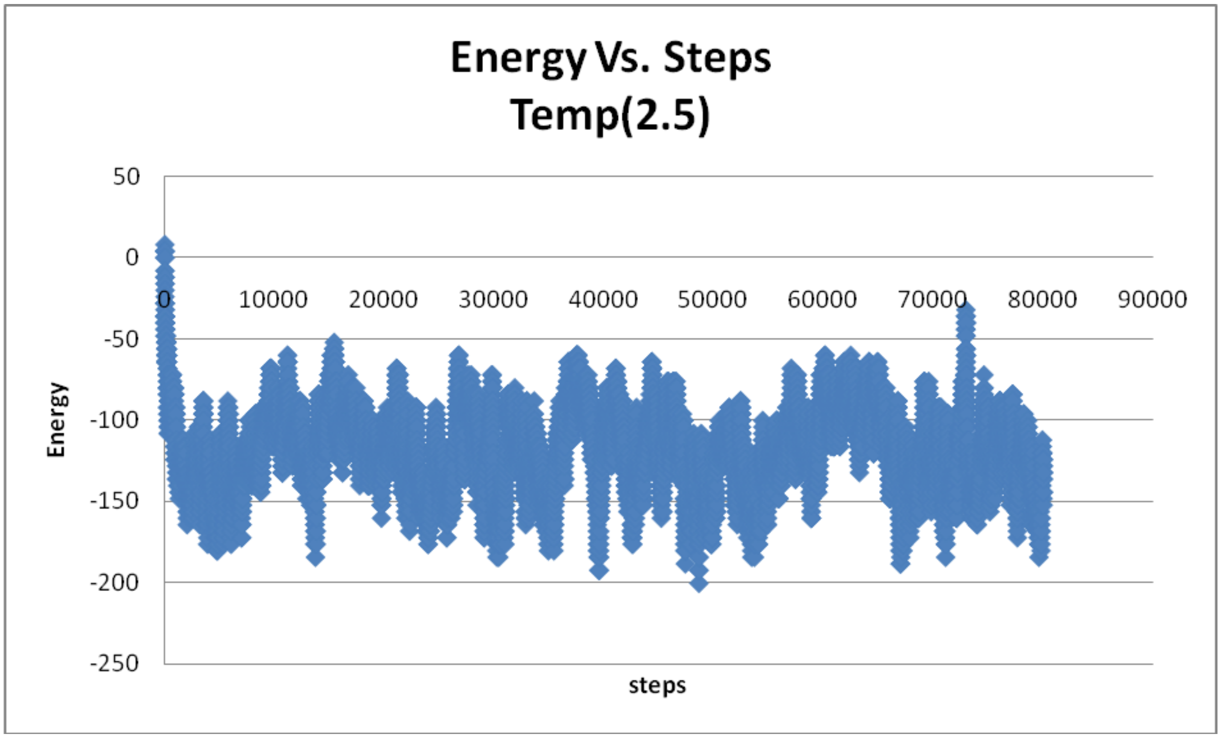
Temperature: 2.5

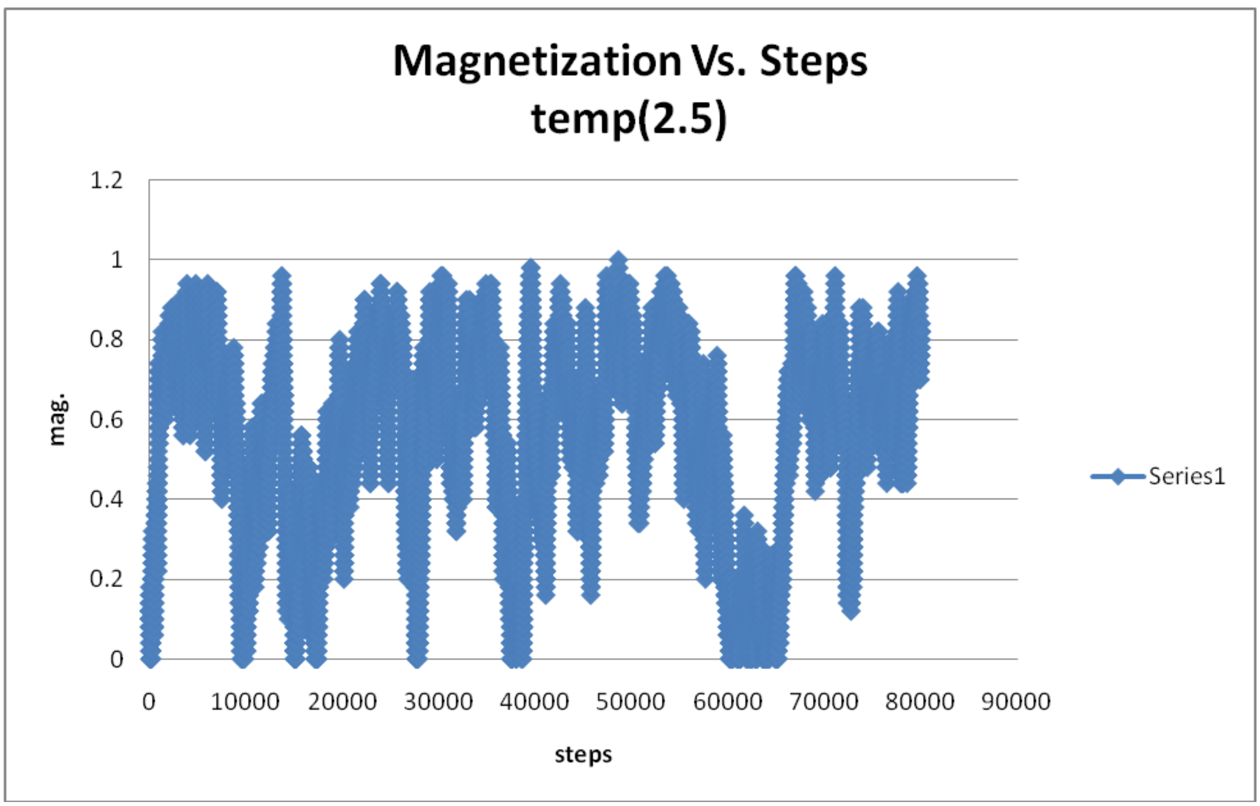
Spin map: initial final





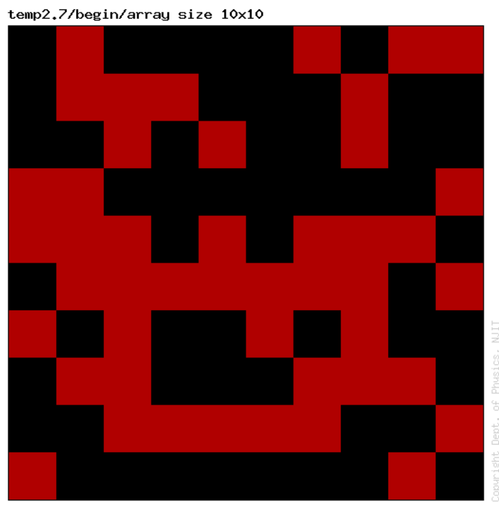
Excel Data plots



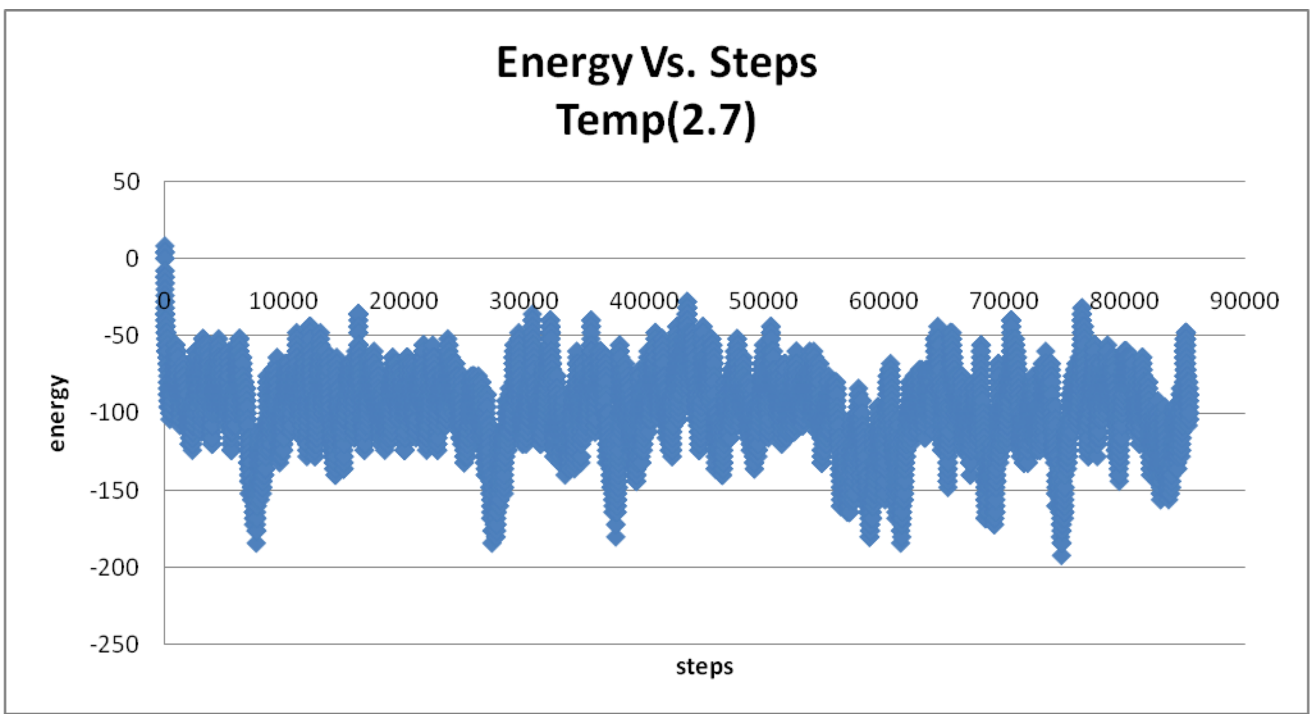


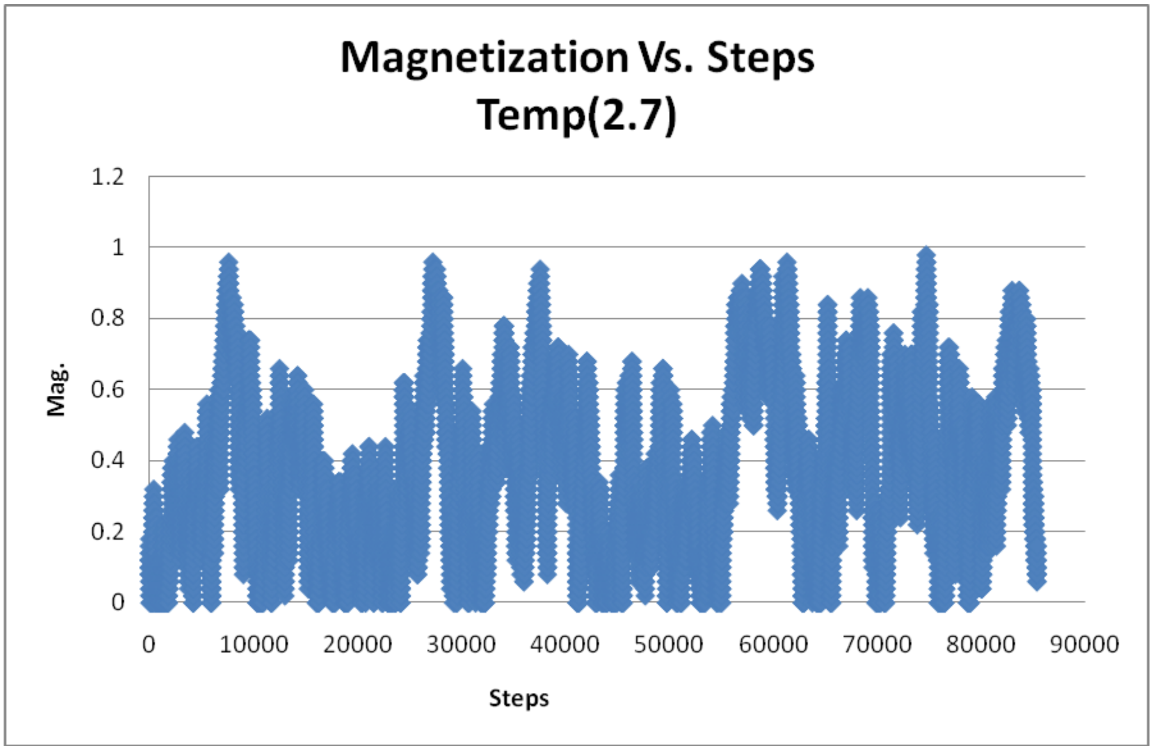
Temperature: 2.7

Spin map initial **final**



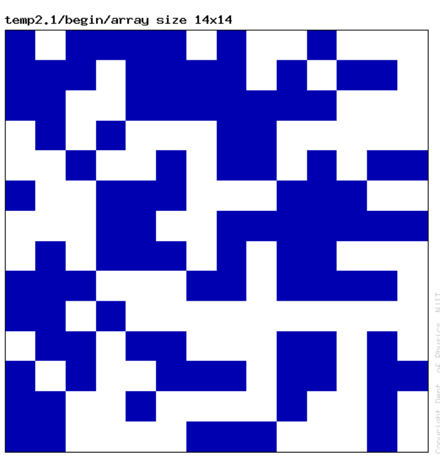
Excel Data plots

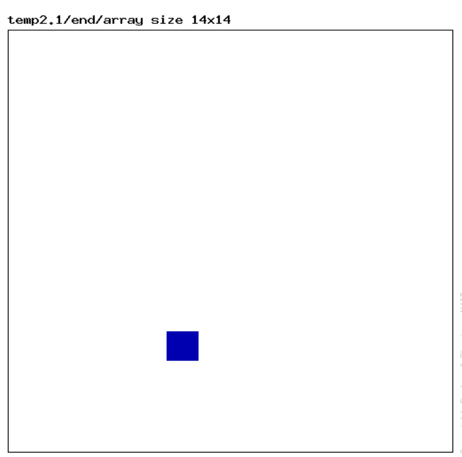




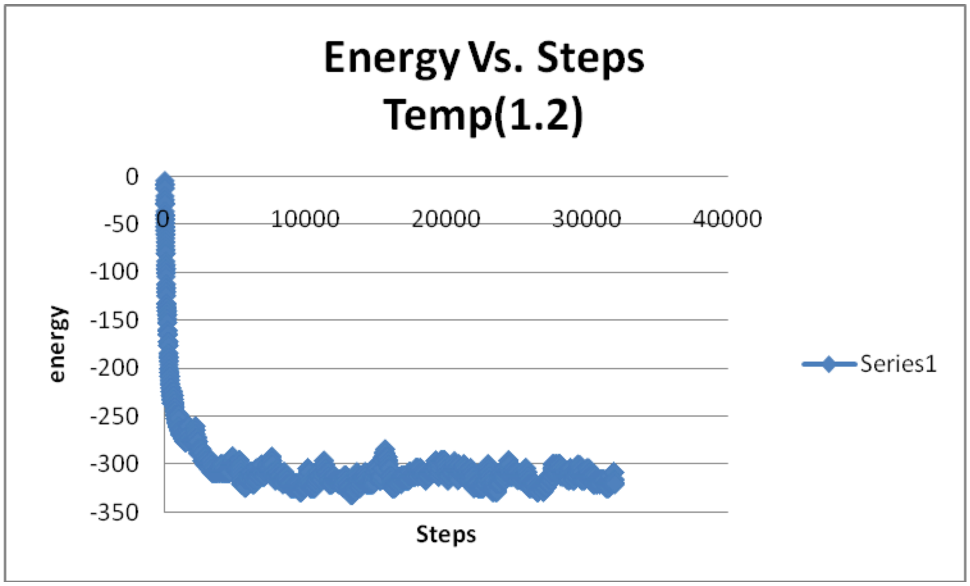
A System with array size of 14 x 14, Temperature: 1.2

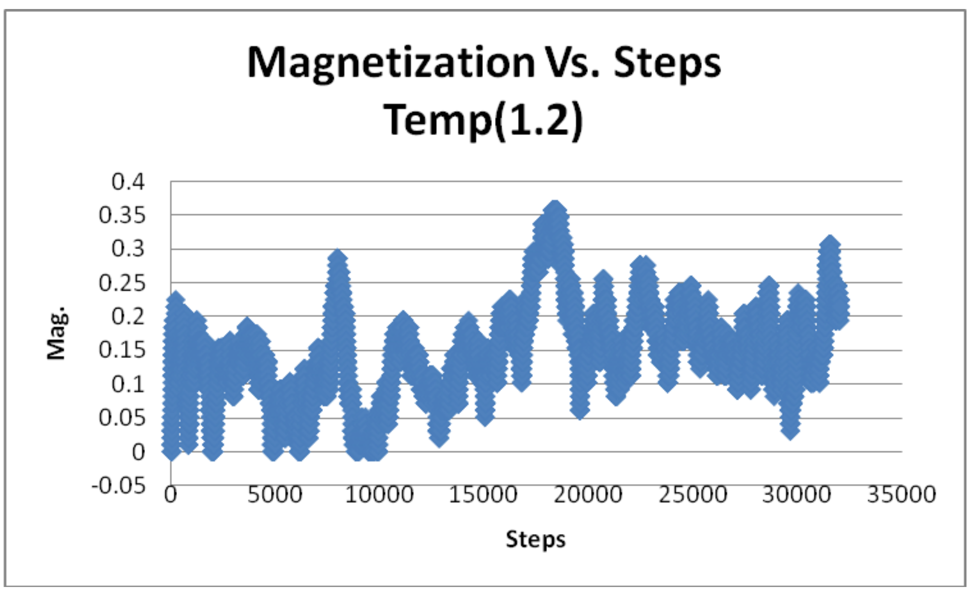
Spin map initial final

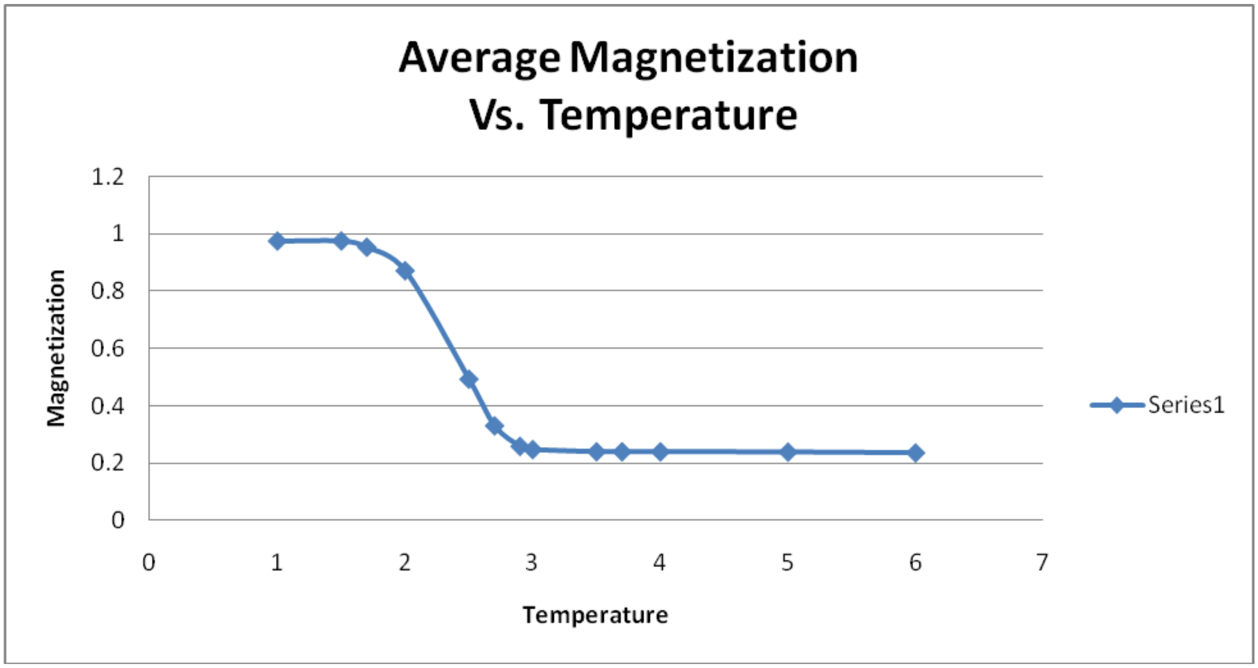




Excel Data Plot







Discussion

We calculated the percentage error for the magnetization graph to compare the observed value (2.7) to the accepted value of the curve which is 2.6. The percentage error resulted in 11.53%. At our observed point, thermal equilibrium occurs.

Conclusion

In conclusion, the whole research was successful. Although our tested system didn't reach absolute zero, the system did what it was ordered to do. The c++ computer simulation gave reasonable results, having a percentage error of 11.5% on the magnetization Vs. Temperature graph.

Acknowledgments

I would like to thank both mentors, Dr. Ken Ahn and Tsezar F. Seman for all there help and support during the course of the summer program. We successfully accomplished how goals in the research. I gained experience in advance studies and developed a greater interest in scientific areas. I would also like to thank Ms. Susan Fahrenholtz and the ACS community for giving me an opportunity to do this program for that second time around.

Appendix

```
//2D Ising Model
//Shenelle Alleyne
//08/04/09

// implements fucntions that will find the energy and magnetism of a 2D system.
// the array size of the system is 10 by 10.
//temperature is introduce in order to see fluxuation in the energy
//and magnetization graphs.

#include <iostream>
#include <cstdlib>
#include <fstream>
#include <cmath>
#include <stdio.h>

using namespace std;

#define NX 10
#define NY 10


// function calculating the energy
double Energy(int dom[][NX])
{

        int row, col, ir, ic;
        double energy = 0.0;
        for(row = 0; row < NY; row++) {
                for(col = 0; col < NX; col++) {
                        // periodic boundary condition
                        if(row == NY-1) ir = 0;
                        else ir = row + 1;
                        if(col == NX-1) ic = 0;
                        else ic = col + 1;

                        energy = energy + dom[row][col] * (dom[row][ic] + dom[ir][col]);
  }
        }

        return -1.0 * energy;
}

/////////////////////////////////////
// spin initializaiton
//
void initialize(int dom[][NX])
{
        int row, col;
```

```
	for(row = 0; row < NY; row++)
	{
		for(col = 0; col < NX; col++)
		{
			if(rand() < RAND_MAX/2)
				dom[row][col] = 1;
			else
				dom[row][col] = -1;
		}
	}
}
////////////////////////////////////

// fuction to save spin array
void savespinstate(int dom[][NX], char* filename)
{
	ofstream fout;
	fout.open(filename);

	int row, col;
	for(row = 0; row < NY; row++){
		for(col = 0; col < NX; col++) {
			fout << dom[row][col];
			if (col < NX-1) fout << ",";
		}
		fout << "\n";
	}
	fout.close();
}

//////////////////////////////////////
// magnetization function
double mag(int dom[][NX])
{
     int row, col;
     int mag = 0;
          for(row = 0; row < NY; row++) {
         for(col = 0; col < NX; col++) {
              mag += dom[row][col];
         }
     }
     if(mag < 0) mag = mag * -1;
     return (double)mag / (NX*NY);
}

/////////////////////////////////////

//rand() genterator
```

```
double unitrand()
{
     return (double)rand() / RAND_MAX;
}
///////////////////////////////////


int main()
{
            double E_old, E_new;
            int dom[NY][NX];
            int r, c;
            int steps = 0;
            int E_gr = -(1*2*NX*NY);
            int counter = 0;
             double prb;
             double T=1.2;

             srand(7);

            // intitialize spins
            initialize(dom);

//saves 2D spinstate in file
savespinstate(dom, "spinsT1.2_begin.txt");

 //fout text file that saves the energy and magnetization values
ofstream fout_en("2DspinsT1.2.txt", fstream::out);
ofstream fout_mag("2DmagT1.2.txt", fstream::out);

   E_old = Energy(dom);

   while ( steps < 50000)
            {
                        r = rand() % NY;
                        c = rand() % NX;

                        dom[r][c] = -1 * dom[r][c];

                        // calculates new energy
                        E_new = Energy(dom);

       double De = (E_new - E_old);

       if(De <= 0)
        {
            E_old = E_new;
            fout_en << steps << "\t" << E_old << "\n";
```

```
            fout_mag << steps << "\t" << mag(dom) << "\n";
        }
            // else statement calculating probability
            else
            {
                prb = exp(-De/T);
                if (prb > unitrand())//(newEnergy <= oldEnergy)
        {
            E_old = E_new;
            fout_en << steps << "\t" << E_old << "\n";
            fout_mag << steps << "\t" << mag(dom) << "\n";

        }
            else
            {
                dom[r][c] = -1 * dom[r][c];
                fout_en << steps << "\t" << E_old << "\n";
                fout_mag << steps << "\t" << mag(dom) << "\n";
                            }
    }
        steps++;
    }
            fout_en.close();
            fout_mag.close();
           //saves 2D spinstate in file
            savespinstate(dom, "spinsT1.2_end.txt");
            system("PAUSE");
            return 0;
}
```

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