Project SEED

Ferromagnetism and Curie Temperature Observed by the Modeling of Exchange Interactions on the Atomic Scale through the Ising Model and the Monte Carlo Technique with C++ Programming

A Conclusive Report
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USA

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I. Introduction

Over this summer, I, along with two other students, were able to recreate and partake in the rediscovery of Curie point temperature. Curie point is a temperature that is unique to every element prone to magnetization; this concept will be explained under theory. The application of this theory is incredible and has allowed us closely study ferromagnetism and properties of elements. What we recreated, from our own deduction and guidance by our mentors, was the Ising Model. It is a simulation of a two dimensional lattice of atoms. We are able to draw information such as energy, magnetization, and spin maps from the lattice. Along with this, we are to input temperature. Thus, we have all of the elements necessary to study how atoms interact and change under different temperatures, as well as being able to observe changes in energy and magnetization.

II. Theory

To brush up on some of the theory behind the project, I have compiled several reports and research that have incremented throughout the course of the program.

Phase Transition

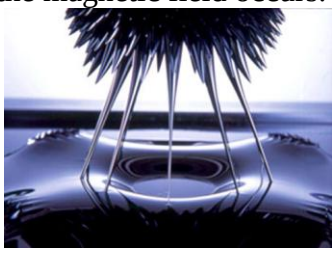
As materials rise and fall through different temperatures, they are susceptible to change in state. The four states of matter are solid, liquid, gas, and plasma. The phase transitions for solids and liquids are freezing and melting. For liquids and gases they are vaporization/evaporation and condensation. For gases and solids they are deposition and sublimation. Plasma only transition from gas and only to gas, the processes are called ionization (to plasma) and deionization (from plasma). A material's state does not only depend on temperatures, but also on pressures. This can be explained through the combined gas law, more specifically Gay-Lussac's Law. This law states that the temperature and the pressure that a material is under are directly proportional. Thus, materials react to pressure changes as they would temperature changes, if mass and volume remains the same. Many take hold of phase transitions and use them in science. In thermodynamics, physicists try and harness energy from heat through chemical processes and phase changes.

- Second Order Phase Transitions - Ferromagnetic Phase Transition

Ferromagnetic phase transitions are second-order phase transitions. They do not have much to do with latent heat like the phase transitions above. This is a transition caused by Curie temperature, when a ferromagnet is no longer magnetic, of when a ferromagnet becomes magnetic. The transition is caused by too much kinetic energy present for the electron spins to allign. With increased entropy, the ferromagnet cannot stay organized and magnetized.

Ferromagnetism

Ferromagnetism is the process under which certain materials become permanent magnets. It is associated with iron, cobalt, nickel, and some alloys or compounds containing one or more of these elements and also a few rare earth elements. Ferromagnets are electrically uncharged and used in electric motors, generators, transformers, telephones, and loudspeakers. Ferromagnetic materials have a unique ordering characteristic in which unpaired electron spins line up parallel with one another, creating a region called a domain. The domain is the area where dipoles are and where the magnetic field occurs.


Ferromagnetic liquid (field, top bulb, is created by application of an outside field)

Electron Spin

Three properties of an electron are charge, mass and spin. The spin is an intrinsic characteristic of electrons and many particles. This spin gives an electron some of its magnetic properties. A charge that moves, or spins, creates a magnetic field. This is how spin is measured; the interaction between an outside magnetic field and the electron is measured. Some would say that electrons behave like little tops! Strong magnetic fields are caused by electron spins aligning.

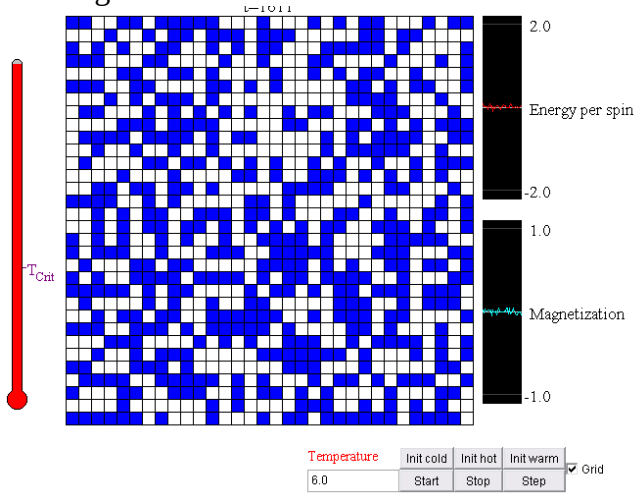
Curie Temperature

When heated to a certain temperature called the Curie point, which is different for each substance, ferromagnetic materials lose their characteristic properties and cease to be magnetic; however, they become magnetic again when they cool. This temperature is named after Pierre Curie, who studied magnetism and radiation. He discovered that substances have a critical temperature where their ferromagnetic behaviors change, this temperature is referred to as Curie point or temperature. When a ferromagnet is below Curie point it has magnetic properties. The phenomenon of what happens past Curie point is caused by the kinetic energy of the atoms; as they rise in entropy, they combat with the dipoles of the material to stay aligned. As the temperature increases, the alignment approaches chaos (entropy) and the field is dispersed.

Ising Model

Named after Ernest Ising, this model has been used to model ferromagnetism. It considers the interactions of spins between particles in materials. In an Ising model, a spin is either point up or down, these are states of objects in Ising models. The model describes the energies of each possible “state”, which are up(white) or down(blue). This

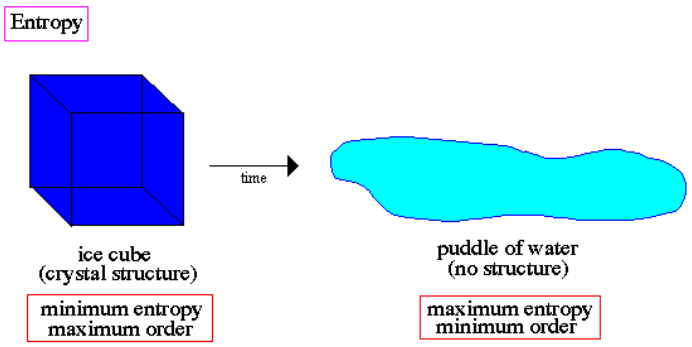
helped to observe and compare the model to actual fluctuations of ferromagnets near Curie point. The model also takes into account temperature, linking temperature, energy, and magnetization.



2 dimensional Ising model

Absolute Temperature

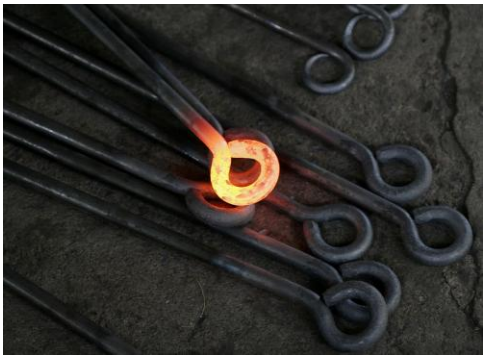
Temperature is a measure of the average kinetic energy of a substance, the warmer, the greater the energy. Simply put, it is a measure of the amount of movement that the atoms of a material are makig. The kinetic energy is created through the molecules and/or atoms of a substance moving and vibrating. So, the colder a substance is, the less movement goes on, there is more order. On the other hand, as a substance increases in temperature, there is less order. This can be described as chaos. The random arrangement in a gas is chaotic compared to the order of a solid state. If something is very chaotic, then it has a high amount of entropy. Entropy is a measure of chaos in a system. There is always entropy present, unless molecules and atoms are not moving enough to affect one another. If this occurs, there is zero entropy, and thus a substance is at absolute zero.



There is no kinetic energy being transferred between molecules and atoms. This temperature is zero on the Kelvin scale and -273.15 Celsius. This temperature is closely studied in cryogenics and is actually artificially and naturally impossible to create. Many triumphs in absolute zero were made and created by William Thompson (Lord Kelvin). The closest natural temperature to absolute zero is -272 ° C, or 1 Kelvin. This is the Boomerang Nebula in the Centaurus Constellation. It is colder than the background radiation of the Big Bang, which is -270 ° C.

Energy

Energy is the amount of work that can be or is performed by a force, it is a scalar quantity based on displacement and points of reference. Work is the amount of energy transferred by a force, a change in energy applied by a force. There are different types of energy that are all named depending on the force doing the work. They are kinetic, potential, thermal, gravitational, sound, light, elastic, and electromagnetic energies. All of these energies have work in common, thus they can be transformed from one to the other. Another characteristic of energy is that it is always conserved. This is the law of conservation of energy. This states the total energy within an isolated system remains constant, thus energy cannot be created or destroyed, though it can change form; an example of this would be a conversion of potential to kinetic to thermal. (Heat is both potential and kinetic)



Exchange interaction/energy

Exchange interactions are interactions between two or more identical particles. In ferromagnetic materials, these interactions are spin-spin interactions for exchange interactions tend to align neighboring spins. These interactions thus create small regions that are magnetized, now observed as magnetic domains. Exchange interactions are quantum mechanical effects, thus they are not results of any forces. They are the results of wave functions of indistinguishable particles, such as two electrons, being open to exchange symmetry. This states that no physical quantity will change after the exchanging of two identical particles. The spins of the two particles might also be identical, if the wave functions of the particles are symmetrical to each other; if the wave functions are anti-symmetrical, the spins of the electrons become opposite. If the electrons are parallel in position and spin, then they are magnetized, and thus this is the cause of ferromagnetism in materials such as iron. If the later happens, the electrons are anti-symmetrical, their spins are anti-parallel, causing anti-ferromagnetism in materials. The results of exchange functions are magnetic, but this is not why they happen. They happen due to electric repulsion and the Pauli Exclusion Principle.

Boltzmann Constant

The Boltzmann constant is a number that relates energy at a particle level with temperature. The constant is written as ‘k’ and is the result of the gas constant,

$R = 8.314\,472(15)\ \frac{\mathrm{J}}{\mathrm{K\,mol}}$. , divided by the Avogadro constant, $N_A = 6.022\ 141\ 79(30) \times 10^{23}\ \mathrm{mol}^{-1}$. The result is $1.3806504(24) \times 10^{-23}$ JK ^–1. This is the bridge between macroscopic and microscopic physics through the ideal gas law. Macroscopically, it can be observed that the

$$pV = nRT,$$

product of pressure p and volume V of an ideal gas is proportional to the product of the amount of substance n and Absolute temperature T, introducing the Blotzmann constant transform this formula for macroscopic observations will become one for microscopic $pV = NkT$ observations, where N is number of moles. So now thanks to Boltzmann, the ideal gas law is applicable to both worlds!

III. Method

The methods used to simulate Curie temperature for K = 1 (k is the Boltzmann Constant) were several equations and algorithms that had to be transcribed into C++.

The equation used to calculate energy was

$$E_{2D} = -\sum S_i (S_{i+10} + S_{i+01})$$

The equation used to calculate magnetization was

$$M = \frac{1}{N} \sum S_i$$

S is the spin value at index i.

After we implemented these equations we had to factor in temperature, through probability. For this we used the Monte Carlo Technique, which introduced temperature and uses Boltzmann Distribution. They are a class of algorithms that are used for probability and help to make our random generator appear random enough or experimentation.

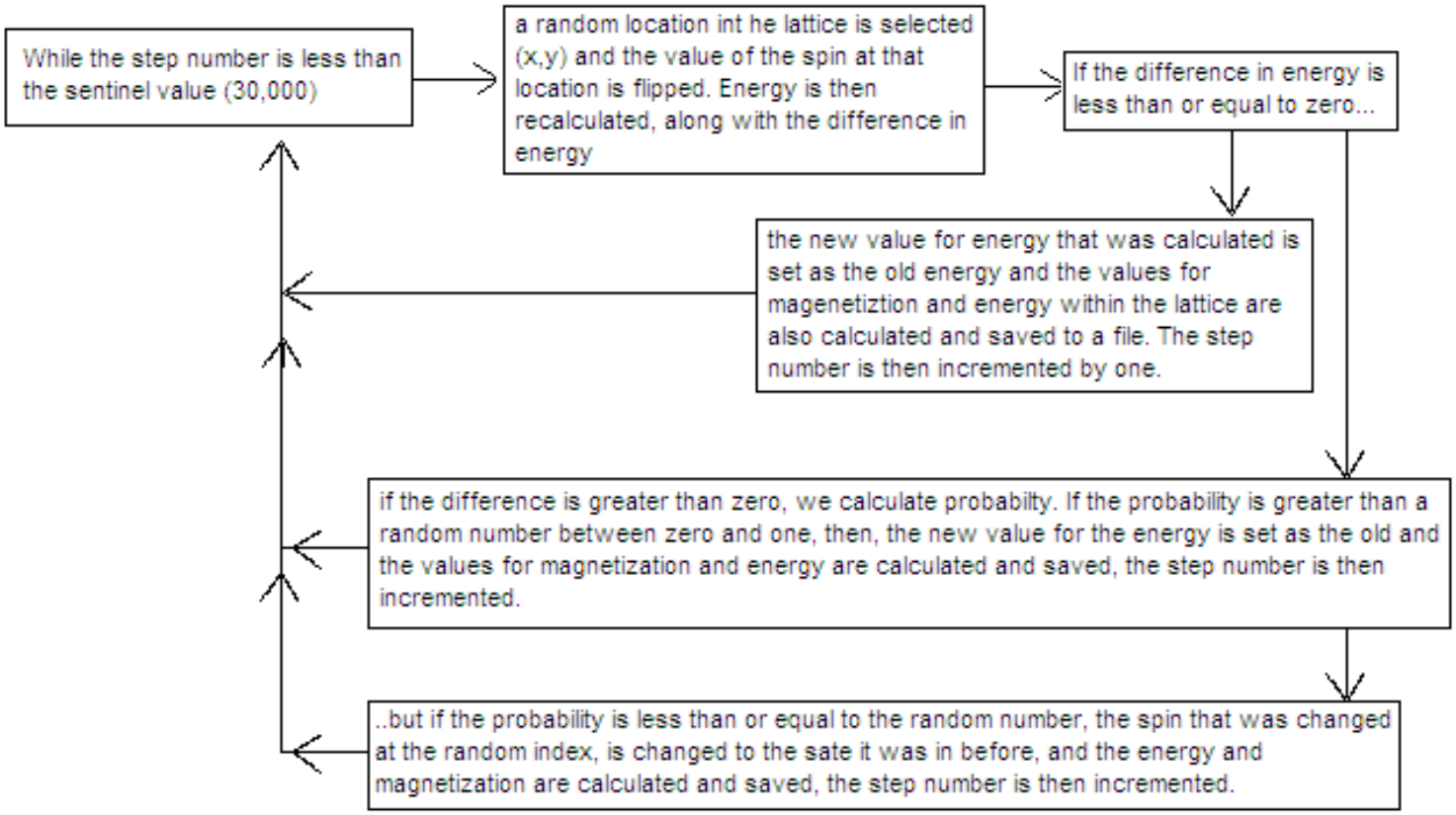
$p = 1 / e^{\Delta E / kT}$ Delta E is the difference in energy every time i increments. K is the Boltzmann constant, which we set to 1 here. T stands for temperature.

Here is the implementation,

```
while  (steps < 30000)
{
        //selects a random atom
        randNum = rand() % N;
```

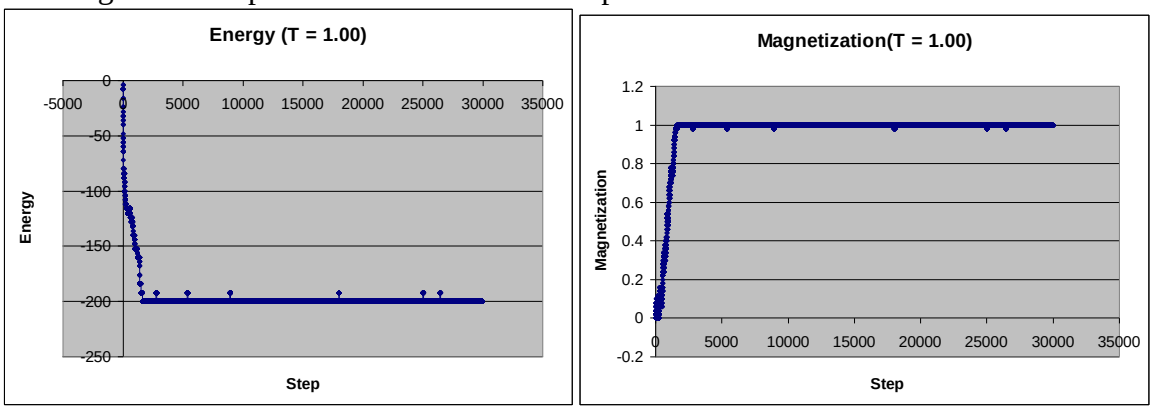
```
        rRow = randNum % NROWS;
        rColumn = randNum / NROWS;
        //switches the spin value at the random location to the opposite value
        ddArray[rRow][rColumn] = -1 * ddArray[rRow][rColumn];
        //calculates energy
        newEnergy = calcEnergy(ddArray);
        //calculates the difference in energy after a spin is changed
        dE = newEnergy - oldEnergy;


    if(dE <= 0) // tests if the difference in energy is less than or equal to zero
    {
            oldEnergy = newEnergy;      //sets new energy to old energy
            en_fout << steps << "\t" << oldEnergy << "\n"; //saves energy and magnetization
            mag_fout << steps << "\t" << calcMagnetization(ddArray) << "\n";
    }

    else
    {
        p = exp(-dE/T); //defines probability

        if (p > randomN())
        {
                    oldEnergy = newEnergy;
                    steps++;
                    en_fout << steps << "\t" << oldEnergy << "\n";
                    mag_fout << steps << "\t" << calcMagnetization(ddArray) <<
"\n";
         }
         else
        {
                   ddArray[rRow][rColumn] = -1 * ddArray[rRow][rColumn];
                    en_fout << steps << "\t" << oldEnergy << "\n";
                    mag_fout << steps << "\t" << calcMagnetization(ddArray) <<
"\n";
        }
            //saves probability values for trouble shooting is needed
            fout << steps << "\t" << p << "\n";
            steps++; //increments steps
}
```

Here is a map of how the code works.

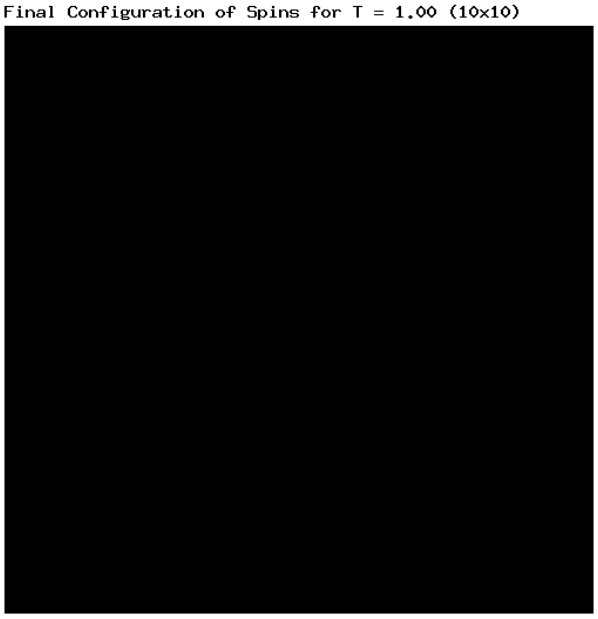


IV. Results

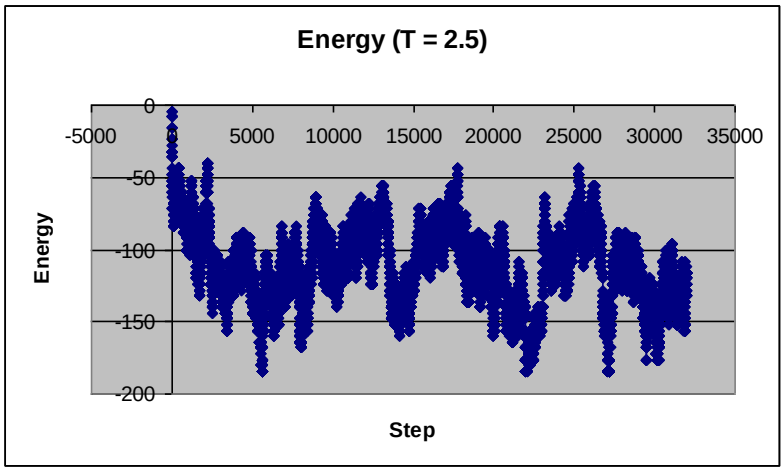
The results for the loop above were very interesing. We took the average magnetizations of different tempertures that we input and plotted them. This gave us a curve of average magnetization versus temperature. Before we see those plots, we should see the Energy and Magnetization plots for three different temperatures.



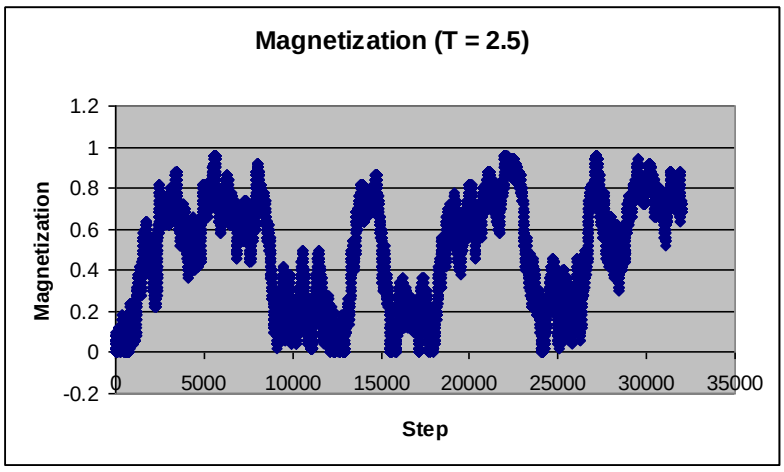
The energy plot shows us that the value for energy within the lattice at Temperature = 1.00 is very low. Subsequently, the magnetization is very high, for the atoms are very organized and stagnant.



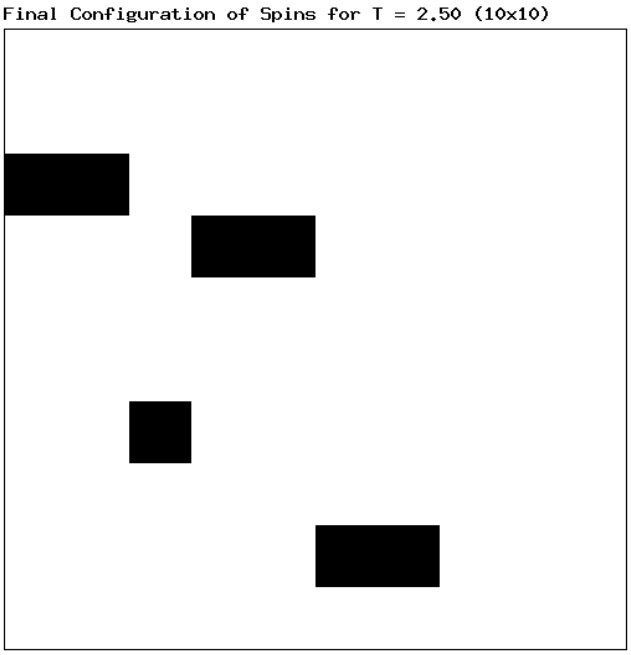
We can see that the lattice was able to reach ground state energy. All of the spins are alligned, explaining the solid color. In this Spin map are one hundred atoms, they are all colored black because all of their electron spins are facing downwards. This results in a huge magnetization.



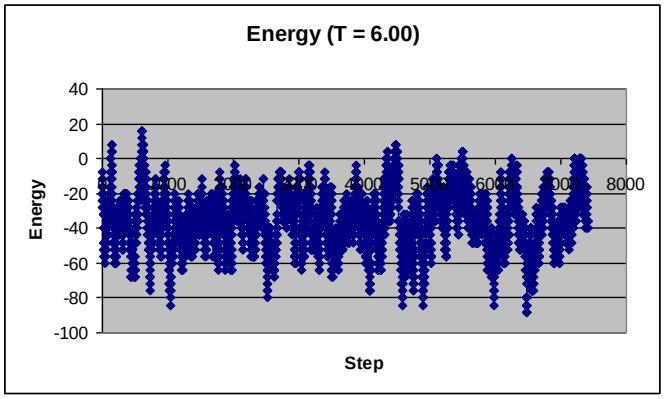
For T = 2.5, we see that there is energy fluctuation and a lot less order. The increase in temperture added more energy to the lattice. The energy is measured by the exchange interactions between every single atom.



The plots are very similar, where energy decreases, magnetization increases. With more temperture, there is more entropy. The energy is too great for the spins to stay alligned.

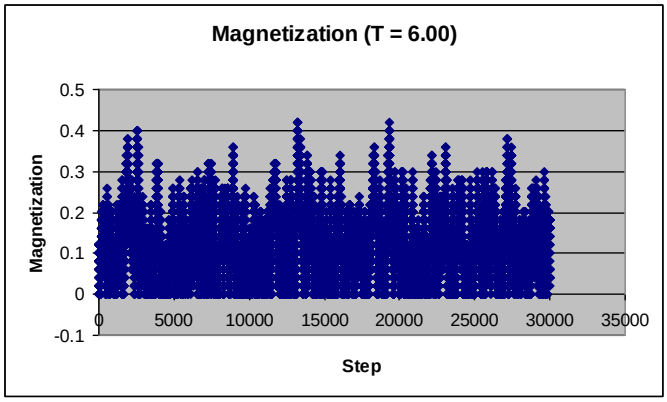


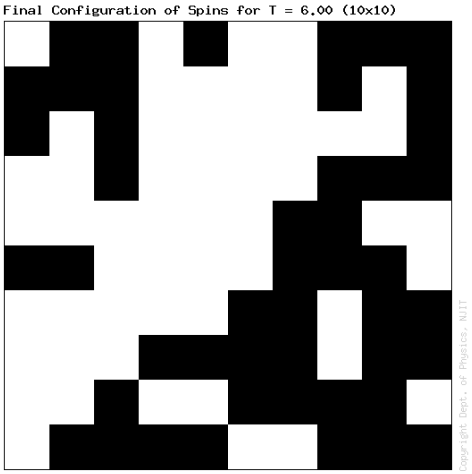
Here we see the struggle for order as the added temperture changes the values of the spins. This is a transition from order to chaos as we increase temperature gradually. Next are the plots for T = 6.00.



Now we see a great increase in energy. After a certain temperature point, which is unique for ever substance, Order is lost and magnetization cannot exist, this temperature is called Curie point and we pinpointed the temperature byfinding the averages of magnetization for many temperatures

Magnetization ofcourse corresponds with the energy and as we can tell, the average is between .1 and .2, a very low magnetization. There is way too much energy for the spins to stay put.

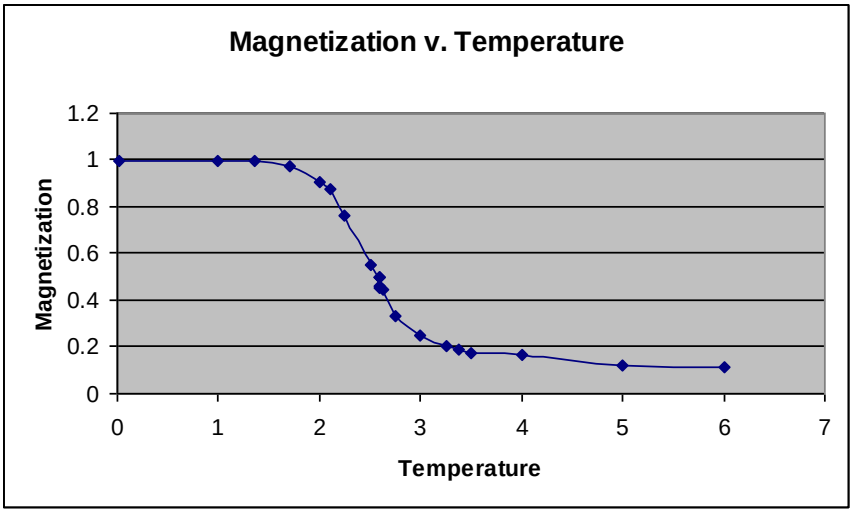




As we can see, there is a lot of chaos in the lattice now. By the end of the simulation, there is no order and the energy has a very high average (-35.9952). The ground state energy would be -200. This is because according to the equation we use, if all of the spins have the same value, (as they would at ground state), the energy would equal -200.

$$E_{2D} = -\sum S_i (S_{i+10} + S_{i+01})$$

This plot is the product of all of our reasearch. We see that while the boltzmann constant is one, a substance loses magnetization at a point between two and three.



Temperature	Magnetization
0.01	1
1	0.999846
1.35	0.993331
1.7	0.973404
2	0.904064
2.1	0.874052
2.25	0.759562
2.5	0.554337
2.5961	0.498015
2.5969	0.495452
2.597	0.495452
2.599	0.459075
2.6	0.449472
2.625	0.445128
2.75	0.333168
3	0.252508
3.25	0.205806
3.375	0.186442
3.5	0.172703
4	0.168378
5	0.122496
6	0.112622

The specific value for Curie Temperature here is 2.5961. It is the lowest value, that could be calculated with the precision allowed by Microsoft Excel, that had a value under 0.5 magnetization. Specifically the value for it's magnetization is 0.498015

V. Discussion

The accepted value for Curie Temperature in a two dimensional model is 2.269J.

((2.5961-2.269) / 2.269) * 100 = 14.416% error.

As we rise in temperatures, magnetization lowers. The trend you see above is for a ten by ten lattice. If you were to say increase the dimensions, the magnetizations would scale with the increase. This is because there are more elements and more room for a spontanenous event to occur. Thus you can make magnetiztion smaller above Curie Temperature by making the lattice smaller.

What one might also notice is that magnetization does not become zero or disapear after Curie Point is reached in the simulation, while in real life, magnetism in

materials disappears after this point. What the two dimensional Ising Model ignores is that electron spins may not only be up and down, but also left right, backwards, forwards, and every angle in between. Beyond Curie point in real materials, there are too many possibilities, ups downs, lefts rights, backwards forwards, that magnetization is impossible to induce or expect.

VI. Conclusion

When first reasearching all of these concepts, one could be dumbfounded. With many conepts that had to be taught from the ground up, the process that was implemented in order to learn and rediscover Curie Temperature was great.

Even though my program had 14% error, the curve matched those of other studies. The large error might have been in part by the psuedo random generator that C++ implements.

In conclusion, the energy, magnetization, and configuration of a system of atoms are greatly dependent on the temperature. The phenomenon known as Cruie Temperature is very interesting for it is a testament to the sensitive of nature. It also allows us to study magnets, the creation of magnets, and magnetic extremes about one of the most important objects to us today.

VII. Acknowledgement

My gratitude goes out to my professors Dr. Ken Ahn, Tzesar F. Seman and my fellow students Mayrolin Garcia and Shenelle Alleyne. Everyone was a great help along the way, as I hope I was. This experience allowed me to make several friends and professors to come visit if I am ever around NJIT. Thank you for a great summer, I learned a lot and I owe it to everyone.

VIII. Appendix

```
// finalVersionCurieTemp.cpp - Alibek Medetbekov
#include <iostream>
#include <fstream>
#include <cmath>
#include <string>
#include <stdio.h>
#include <string.h>
#include <iomanip>

using namespace std;
//declaration of the size of the lattice
const unsigned int NROWS = 10, NCOLS = 10;
const unsigned int N = NROWS * NCOLS;

void save (char* pFile, int domain[][NCOLS]) //saves cofiguration of
lattice electron spins
{
        int i, j;
        ofstream fout;
        fout.open(pFile, fstream::out);

        for(i = 0; i < NROWS; i++)
        {
                for(j = 0; j < NCOLS; j++)
                {
                        fout << domain[i][j];
                        if (j != NCOLS-1)
                                fout << ",";
                }
                fout << "\n";
        }
        fout.close();
```

```
}

double randomN() //generates a random number between 0 and 1
{
	return (double)rand()/ RAND_MAX;
}

void initialize(int domain[][NCOLS]) //initializes the array
{
	int i, j;
	for(i = 0; i < NROWS; i++)
	{
		for(j = 0; j < NCOLS; j++)
		{
			if ((double)rand()/RAND_MAX < 0.5)
				domain[i][j] = -1;
			else
				domain[i][j] = 1;
		}
	}
}

double calcMagnetization(int domain[][NCOLS]) //calculates
magnetization
{
	int i, j;
	int magnetization = 0;
	for (i = 0; i < NROWS; i++)
	{
	   for (j = 0; j < NCOLS; j++)
	   {
			magnetization += domain[i][j];
	   }
	}
	if (magnetization < 0) magnetization *= -1;
	return (double)magnetization / (NROWS * NCOLS);
}

double calcEnergy(int domain[][NCOLS]) // calculates energy
{
	int i, j, i_new, j_new;
    double energy = 0.0;
    for(i = 0; i < NROWS; i++)
    {
		for(j = 0; j < NCOLS; j++)
		{
			if (i == NROWS-1) i_new = 0;
			else i_new = i + 1;
			if (j == NCOLS-1) j_new = 0;
			else j_new = j + 1;

			energy += domain[i][j] * (domain[i][j_new] +
domain[i_new][j]);
		}
    }
    return -1.0 * energy;
}
```

```
int main()
{
        int steps = 0;
        int ddArray[NROWS][NCOLS];
        double newEnergy, oldEnergy, p, pOld, T = 2.5961, dE, totalMag =
0.0;
        int rRow, rColumn, randNum;
    double e_Gr  = -2.0 * (double)N;

    // starts streams that will save the data
        ofstream en_fout("2DEnergy.txt", fstream::out);
        ofstream mag_fout("Magnetizations.txt", fstream::out);
    ofstream fout("probability.txt", fstream::out);
    ofstream avgMag_fout("avgMag.txt", fstream::out);
        initialize(ddArray);
        save("initial2DConfiguration.txt", ddArray);


        oldEnergy = calcEnergy(ddArray);

        en_fout << steps << "\t" << oldEnergy << "\n";
    //random seed (in order to repeat experiements with the same random
numbers)
        srand(876);
    //begining of loop
        while  (steps < 60000)
    {
                //selects a random atom
            randNum = rand() % N;
                rRow = randNum % NROWS;
                rColumn = randNum / NROWS;
                //switches the spin value at the random location to the
opposite value
                ddArray[rRow][rColumn] = -1 * ddArray[rRow][rColumn];
            //calculates energy
            newEnergy = calcEnergy(ddArray);
            //calculates the difference in energy after a spin is
changed
            dE = newEnergy - oldEnergy;

            if(dE <= 0) // tests if the difference in energy is less
than or equal to zero
            {
                        oldEnergy = newEnergy;      //sets new energy to
old energy
                        en_fout << steps << "\t" << oldEnergy << "\n";
//saves energy and magnetization
                        mag_fout << steps << "\t" <<
calcMagnetization(ddArray) << "\n";
            }
            else
            {
                    p = exp(-dE/T); //defines probability
                    if (p > randomN())
                    {
                                oldEnergy = newEnergy;
```

```
                                    steps++;
                                    en_fout << steps << "\t" << oldEnergy
<< "\n";
                                    mag_fout << steps << "\t" <<
calcMagnetization(ddArray) << "\n";
                        }
                        else
                        {
                                ddArray[rRow][rColumn] = -1 *
ddArray[rRow][rColumn];
                                    en_fout << steps << "\t" << oldEnergy <<
"\n";
                                    mag_fout << steps << "\t" <<
calcMagnetization(ddArray) << "\n";
                        }
                        //saves probability values for trouble shooting is
needed
                                fout << steps << "\t" << p << "\n";
                                steps++; //increments steps
            }
    }
    save("final2DConfiguration.txt", ddArray);
    avgMag_fout << totalMag/(double)steps;
        en_fout.close();
        mag_fout.close();
    avgMag_fout.close();
    fout.close();

        system("PAUSE");
        return 0;
}
```

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