



**Sudan University of Science & Technology (SUST)**  
**College of Graduate Studies**  
**Faculty of Science-Department of Physics**



## **Effect of High Temperature on Phase Transition of Nickel Oxide (NiO) by Simulation Using Ising Model**

**تأثير درجة الحرارة العالية على تحول الطور لأكسيد النيكل بالمحاكاة  
باستخدام نموذج أيزينج**

**A Thesis Submitted in Partial Fulfillment of the Requirements  
For the Degree of Master of Science in Physics**

**By**

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## *Dedication*

*I dedicated this research to my parent's soul.*

# *Acknowledgement*

*First I wish to express my gratitude to my supervisor Dr. Abdelnabi Ali Elamin for dedicated and enthusiastic supervision and for always taking the time to discuss scientific problems pertaining to my research. His personal involvement in all aspects of my research have been very motivating and helpful.*

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*I offer my special gratitude to my brother Elmala for correction grammar errors in chapter one, three and four.*

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## Abstract

In this research had been studied the simulation effect of higher temperature on physical properties such as the critical temperature ( $T_c$ ), the magnetization per spin ( $M$ ), the energy per spin ( $E$ ), the magnetic susceptibility ( $\chi$ ), the specific heat ( $C_v$ ) of NiO for a 6X6 square lattice in the absence of external magnetic field. The simulation results showed that the magnetization per spin changed from a positive value to a negative value at critical temperature  $T_c \approx 47.2679045 \text{ J/K}_B$  this indicates that the material transited from Antiferromagnetic to diamagnetic state. Also, the ground state energy of NiO was determined to be  $-38.125 \text{ meV}$ .

## المستخلص

في هذا البحث دُرس محاكاة تأثير درجة الحرارة العالية على الخواص الفيزيائية مثل درجة الحرارة الحرجة والطاقة والمغناطيسية لكل عزم مغزلي والقابلية المغناطيسية والحرارة النوعية لشبكة أكسيد النيكل المربعة  $6 \times 6$  في غياب المجال المغناطيسي الخارجي. لُوحظ من نتائج المحاكاة أن المغناطيسية لكل عزم مغزلي تغيرت من القيمة الموجبة إلى القيمة السالبة عند درجة الحرارة الحرجة  $T_c = 47.269045 \text{ J/K}_B$ ، وهذا يشير إلى أن المادة تحولت من الحالة الفيرومغناطيسية المضادة إلى الحالة الدايا مغناطيسية. وأيضاً حدد مستوى الطاقة الأرضي لمادة أكسيد النيكل عند  $-38.125 \text{ meV}$ .

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# Chapter One

## Introduction

### 1.1 Introduction

Many physical substances undergo phase transitions when subject to changes in environmental parameters [1]. Phase transitions are common in physics and familiar in everyday life, the transition of ice into water and water into steam are familiar examples [2]. Similarly, Nickel Oxide (NiO) undergoes a phase transition at a specific temperature, that changing its magnetic order from the antiferromagnetic (AF) to the paramagnet state. This magnetic reordering is accompanied by a change in temperature. In other words, the phase transition is a magnetoelastic phenomenon. In this thesis, we study the phase transition of Nickel Oxide (NiO) by directly simulate the effect of temperature on its structure. Several important thermodynamic concepts will also be navigated [1].

The square-lattice Ising model is the simplest system showing phase transitions (i.e. the transitions between the paramagnetic and antiferromagnetic (AF) phase). The square lattice Ising model has played a central role in the understanding of phase transitions [3].

### 1.2 Problem Statement

During experimental studies, difficulties in explaining discrepancies between observations and predictions are encountered due to the fact that high-precision measurements of critical parameters can be unavailable or difficult to obtain.

Some of these difficulties are amenable to solutions using simulation methods. The case of analyzing the properties of phase transition (i.e. the

transitions between the paramagnetic and ferromagnetic phase), which is a major problem in experimental studies, is stimulated to make the case.

When using experimental method the following problems must be addressed:

- Experimental studies need special equipment tools in addition to adjusting the experiment to the surrounding environmental conditions.
- Any experimental result is due to the combined effects of all factors, the strengths and contributions each are practically impossible to single out.
- It is difficult to deal with complex theoretical statistical mathematical model.

### **1.3 Objective of the Research**

The main objective of this thesis to simulate the effect of changing in a factor such as temperature on physical properties of Nickel Oxide (NiO).

The work will include a detailed description on determination of critical temperature ( $T_c$ ), magnetization (M), energy (E), magnetic susceptibility ( $\chi$ ) and specific heat of a NiO as a function of temperature.

### **1.4 Aim of the Research**

Phase transition is important in many industrial processes that are sensitive to fundamental physical properties such as magnetic phase transitions

Nickel oxide (NiO) has many uses the primary of which is in steel and alloy manufacturing. It is also used in the ceramics industry, electronics, fuel cells and solar cell [4].

The aim of this thesis to be the first work to investigate the phase transition of antiferromagnetic phase transition for Nickel Oxide (NiO) using  $C^{++}$  simulation.

## 1.5 Literature Review

Phase transition of nickel oxide has been studied using several methods as reported by many researchers. The simulation results have been analyzed and discussed under various deposition conditions as described in many literature reviews.

Great efforts have been made by T. Chatterji et al (2009) to investigate the antiferromagnetic (AF) phase transition and spin correlations in NiO by high-temperature neutron diffraction below and above  $N_T$ .

They showed that AF phase transition is a continuous second-order transition within their experimental resolution. The spin correlations manifested by the strong diffuse magnetic scattering persist well above  $N_T \approx 530$  K and could still be observed at  $T=800$  K which is about  $1.5N_T$ . They argued that the strong spin correlations above  $N_T$  are due to the topological frustration of the spins on a face-centered cubic (fcc) lattice. The Néel temperature is substantially reduced by this process. They determined that the critical exponents  $\beta=0.328 \pm 0.002$  and  $\nu=0.64 \pm 0.03$  and the Néel temperature  $N_T=530 \pm 1$  K. These critical exponents suggested that NiO should be regarded as a 3dXY system.[5].

Study of the critical phenomena of Nickel II Iron III oxide (Ferromagnetic) was determined using Monte Carlo simulation technique by D.A. Ajadi et al (2014). The critical temperature ( $T_c$ ), the magnetization per site ( $\mu$ ), energy per site ( $E$ ), magnetic susceptibility ( $\chi$ ), specific heat of a NiOFe<sub>2</sub>O<sub>3</sub> were determined as a function of temperature for two different square lattices 20x20 and 150x150. The analysis of simulation results indicate that the bipolar magnet with strong tetragonal distortion in external magnetic field applied along the axis resembles the behavior of the two dimensional Ising model on the rectangular lattices. The numerical solution of the model in MATLAB "R2013a" was presented. A Monte Carlo Algorithm known as

Metropolis Hastings Algorithm was used to evaluate the behavior of the lattice and the critical temperature at which the phase transition between NiOFe<sub>2</sub>O<sub>3</sub> and paramagnetic state occurs was noted. The analysis of the results shows that  $T_C = 2.25J/k_B$ , in the absence of external magnetic field. It was observed that above ( $T_C$ ) the material (NiOFe<sub>2</sub>O<sub>3</sub>) becomes a paramagnetic state, and this leads to decreasing in average magnetization and the average Energy increases, while below ( $T_C$ ) the material is in a ferromagnetic state [6].

A considerable work has been done by Danny Bennett (2016) by using the Metropolis algorithm. The solutions to various versions of the Ising model were obtained. The 2D square lattice was initially considered. After successfully using the Metropolis algorithm to update the system, the average energy per spin, average magnetization per spin, specific heat capacity and magnetic susceptibility were plotted as functions of temperature in order to gain information about the system. The ground state energy was determined to be  $-2J$ , as expected, and the Curie temperature was determined to be  $T_C = 2.6 \pm 0.1J/k_B$  in this case, which compares well with the accepted value of  $T_C = 2.269J/k_B$ , and the ground state energy was determined to be  $-2J$ . The triangular lattice was then investigated; the ground state energy was determined to be  $-3J$ , and the Curie temperature was determined to be  $T_C = 4.2 \pm 0.1J/k_B$ . For the 1D system, a phase transition was initially observed, but this was due to a low value of  $J$  used in computations; when a larger value of  $J$  was used, there was no phase transition, which agrees with the theory. The 3D system was investigated and also determined to be ferromagnetic, with a larger Curie temperature of  $T_C = 4.4 \pm 0.1J/k_B$ , and a ground state energy of  $-3J$ . Finally, the methods developed in the previous parts of the project were used to investigate a simplified 2D model of NiO. The ground state was determined to be  $-36.75 \pm 0.01\text{meV}$ , and the ordered state of the system was determined to be antiferromagnetic [7].

## **1.6 Layout of the Research**

This research consists of four chapters, chapter one has the thesis introduction.

An overview of magnetization property and phase transition and their types and characteristics are presented in chapter two. The structure of nickel oxide is also described. The Ising model and the Monte Carlo method are also described in details.

Chapter three describes the simulation process for the effect of temperature on NiO structure.

The result, discussion, conclusion and recommendations are presented in chapter four.

# **Chapter Two**

## **Theoretical Background**

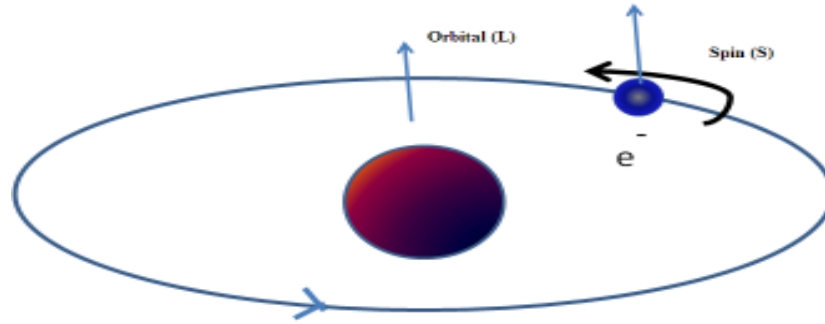
### **2.1 Introduction**

This chapter presents the phenomenon of magnetism and gives in details the types of magnetism. Moreover it also introduces Monte Carlo (MC) techniques as applied in statistical physics which is used for the study of phase transitions of nickel oxide.

Metropolis algorithm (MA), the choice of using the Ising model as a pattern will discuss in details. Also the concept of phase transition and the structure of nickel oxide will discuss in details.

### **2.2 Magnetism**

All matter is magnetic, a phenomenon that is due to the structure of atoms. As is well known from Maxwell's equations, moving charges create magnetic fields. In an atom, an electron has two types of quantum mechanical angular momentum. One is due to orbital motion about the nucleus and the other is due to electron spin, which is a purely quantum mechanical concept. Electron spin is a fundamental property of electrons, and other elementary particles, that forms the basis of quantum mechanics (see figure2.1)[8].



**Figure2.1. Origin of Magnetism**

Each current loop produced by the moving charge of the electron produces its own magnetic moment. However, the spin moment dominates the magnetic behavior of the atom. On average, the magnetic moment due to the orbiting electron will be zero because of the symmetrical motion of the electron around the nucleus. Spin, on the other hand, is a property that is constant for any electron occupying a given quantum state. Because of this orbital magnetic effects do not contribute to the overall magnetic moment of the atom.

In real materials, comprised of many moles of atoms, bulk magnetization effects are observed.

Each of the atoms in the material has its own magnetic moment that contributes to the overall magnetic moment of the material. The total magnetic moment of a material is known as magnetization; magnetization ( $M$ ) is defined as

$$M = \frac{N}{V} \sum_{i=1}^N m_i \quad (2.1)$$

Where  $m$  is the magnetic moment of the  $i$ th particle,  $N$  is the number of particles in the material and  $V$  is the volume over which the sum is computed, normalizing the number to find the average magnetization per spin [8].

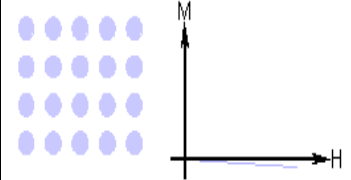
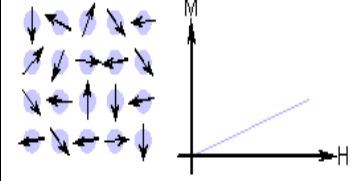
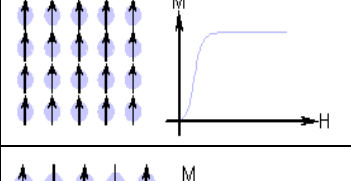
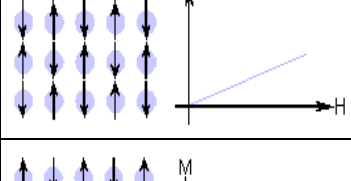
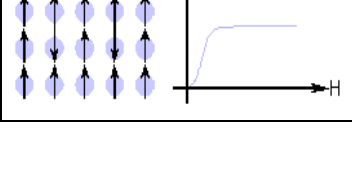
Each material also has an energy associated with the atomic interactions of neighboring dipoles. These interactions, however, are not the same for all materials. In fact, there are several main types of magnetic materials and they

are classified by how their constituent atoms interact with each other and with external magnetic fields [8].

### 2.3 Magnetism Types

The most common classes of magnetic materials are: diamagnetism (DM), ferrimagnetism, antiferromagnetism (AF), paramagnetism (PM), and ferromagnetism (FM) as table illustrated in table 2.1[10].

**Table 2.1.Types of Magnetism**

Type of Magnetism	Susceptibility	Atomic	Magnetic Behavior	Example	Susceptibility
<b>Diamagnetism</b>	Small & negative.	Atoms have no magnetic moment		Au Cu	$-2.74 \times 10^{-6}$ $-0.77 \times 10^{-6}$
<b>Paramagnetism</b>	Small & positive.	Atoms have randomly oriented magnetic moments		$\beta$ -Sn Pt Mn	$0.19 \times 10^{-6}$ $21.04 \times 10^{-6}$ $66.10 \times 10^{-6}$
<b>Ferromagnetism</b>	Large & positive, function of applied field, microstructure dependent.	Atoms have parallel aligned magnetic moments		Fe	$\sim 100,000$
<b>Antiferromagnetism</b>	Small & positive.	Atoms have mixed parallel and anti-parallel aligned magnetic moments		Cr	$3.6 \times 10^{-6}$
<b>Ferrimagnetism</b>	Large & positive, function of applied field, microstructure dependent	Atoms have anti-parallel aligned magnetic moments		Ba ferrite	$\sim 3$

#### 2.3.1 Diamagnetism (DM)

All materials show some degree of diamagnetism, a weak, negative magnetic susceptibility. For a diamagnetic substance, a magnetic field induces a magnetic moment which opposes the applied magnetic field that caused it



[9]. In a diamagnetic (DM) material the atoms have no net magnetic moment when there is no applied field. Under the influence of an applied field (H) the spinning electrons process and this motion, which is a type of electric current, produces a magnetization (M) in the opposite direction to that of the applied field. All materials have a DM effect; however, it is often the case that the DM effect is masked by the larger paramagnetic or ferromagnetic term. The value of susceptibility is independent of temperature.

DM materials have a relative magnetic permeability that is less than 1, and a magnetic susceptibility that is less than 0. (i.e.  $\mu_r = \mu / \mu_o = (1 + \chi_m) < 1$  and  $\chi_m < 0$ ). Diamagnetism was discovered and named in September 1845 by Michael Faraday [10].

### 2.3.2 Paramagnetism(PM)

Paramagnetism corresponds to a positive susceptibility so that an applied magnetic field induces a magnetization which aligns parallel with the applied magnetic field which caused it [9]. There are several theories of paramagnetism (PM), which are valid for specific types of material. The Langevin model, which is true for materials with non-interacting localized electrons, states that each atom has a magnetic moment which is randomly oriented as a result of thermal agitation. The application of a magnetic field creates a slight alignment of these moments and hence a low magnetization in the same direction as the applied field. As the temperature increases, then the thermal agitation will increase and it will become harder to align the atomic magnetic moments and hence the susceptibility will decrease. This behavior is known as the Curie law and is shown below in Equation (2.2), where C is a material constant called the Curie constant.

$$\chi = \frac{C}{T} \tag{2.2}$$

Materials which obey this law are materials in which the magnetic moments are localized at the atomic or ionic sites and where there is no

interaction between neighboring magnetic moments. The hydrated salts of the transition metals, e.g.  $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ , are examples of this type of behavior as the transition metal ions, which have a magnetic moment, are surrounded by a number of non-magnetic ions / atoms, which prevent interaction between neighboring magnetic moments.

In fact the Curie law is a special case of the more general Curie-Weiss law (equation 2.3), which incorporates a temperature constant ( $\theta$ ) and derives from Weiss theory, proposed for FM materials, that incorporates the interaction between magnetic moments.

$$\chi = \frac{C}{T - \theta} \quad (2.3)$$

In this equation  $\theta$  can either be positive, negative or zero. Clearly when  $\theta = 0$  then the Curie-Weiss law equates to the Curie law. When  $\theta$  is non-zero then there is an interaction between neighboring magnetic moments and the material is only paramagnetic above a certain transition temperature. If  $\theta$  is positive then the material is ferromagnetic below the transition temperature and the value of  $\theta$  corresponds to the transition temperature (Curie temperature,  $T_C$ ). If  $\theta$  is negative then the material is antiferromagnetic below the transition temperature (Néel temperature, NT), however the value of  $\theta$  does not relate to NT. It is important to note that this equation is only valid when the material is in a paramagnetic state. It is also not valid for many metals as the electrons contributing to the magnetic moment are not localized. However, the law does apply to some metals, e.g. the rare earths, where the 4f electrons, that create the magnetic moment, are closely bound.

FM materials above the  $T_C$  become paramagnetic. PM Materials, Aluminum, Barium, Calcium, Liquid Oxygen, Platinum, Sodium, Strontium and Uranium [10].

### 2.3.3 Ferromagnetism(FM)

A ferromagnet has a spontaneous magnetization even in the absence of an applied field. All the magnetic moments lie along a single unique direction [9]. Ferromagnetism is only possible when atoms are arranged in a lattice and the atomic magnetic moments can interact to align parallel to each other. This effect is explained in classical theory by the presence of a molecular field within the ferromagnetic (FM) material, which was first postulated by Weiss in 1907. This field is sufficient to magnetize the material to saturation. In quantum mechanics, the Heisenberg model of ferromagnetism describes the parallel alignment of magnetic moments in terms of an exchange interaction between neighboring moments.

Weiss postulated the presence of magnetic domains within the material, which are regions where the atomic magnetic moments are aligned. The movement of these domains determines how the material responds to a magnetic field and as a consequence the susceptibility is a function of applied magnetic field. Therefore, FM materials are usually compared in terms of saturation magnetization (magnetization when all domains are aligned) rather than susceptibility.

In the periodic table of elements only Fe, Co and Ni are FM at and above room temperature. As FM materials are heated then the thermal agitation of the atoms means that the degree of alignment of the atomic magnetic moments decreases and hence the saturation magnetization also decreases. Eventually the thermal agitation becomes so great that the material becomes paramagnetic; the temperature of this transition is the Curie temperature,  $T_C$  (Fe:  $T_C=770^\circ\text{C}$ , Co:  $T_C=1131^\circ\text{C}$  and Ni:  $T_C=358^\circ\text{C}$ ). Above  $T_C$  then the susceptibility varies according to the Curie-Weiss law [10].

### 2.3.4 Antiferromagnetism(AF)

In the periodic table the only element exhibiting antiferromagnetism at room temperature is chromium. Antiferromagnetic (AF) materials are very similar to ferromagnetic (FM) materials but the exchange interaction between neighboring atoms leads to the anti-parallel alignment of the atomic magnetic moments. Therefore, the magnetic field cancels out and the material appears to behave in the same way as a paramagnetic material. Like ferromagnetic (FM) materials these materials become paramagnetic (PM) above a transition temperature, known as the Néel temperature, NT. (Cr: NT=37°C) [10].

### 2.3.5 Ferrimagnetism

Ferrimagnetism is only observed in compounds, which have more complex crystal structures than pure elements. Within these materials the exchange interactions lead to parallel alignment of atoms in some of the crystal sites and anti-parallel alignment of others. The material breaks down into magnetic domains, just like a ferromagnetic (FM) material and the magnetic behavior is also very similar, although ferrimagnetic materials usually have lower saturation magnetizations. For example in Barium ferrite ( $\text{BaO} \cdot 6\text{Fe}_2\text{O}_3$ ) the unit cell contains 64 ions of which the barium and oxygen ions have no magnetic moment, 16  $\text{Fe}^{3+}$  ions have moments aligned parallel and 8  $\text{Fe}^{3+}$  aligned antiparallel giving a net magnetization parallel to the applied field, but with a relatively low magnitude as only  $1/8$  of the ions contribute to the magnetization of the material [10].

## 2.4 Curie Temperature (TC)

Curie temperature ( $T_C$ ) is the temperature at which certain magnetic materials undergo a sharp change in their magnetic properties. They lose their characteristic ferromagnetic ability, 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 too great for them to join together to form small magnetic areas in the material [11]

## **2.5 Phase Transition(PT)**

A Phase transition (PT) is basically a natural physical process [11]it is marked by abrupt macroscopic changes as external parameters are changed, such as an increase of temperature. The point where a phase transition takes place is called a critical point. This section distinguish normally between two types of phase transitions (PT); first-order transitions and second-order transitions [12].

A first order phase transition (PT) is normally accompanied by the absorption or liberation of latent heat, while a second order phase transition has no latent heat. An example of a first order phase transition (PT) is between water and steam (gaseous water), and an example of a second order phase transition that exhibited by is the two dimensional Ising model on a square lattice (magnetization). There is a critical temperature and energy at which the properties of the two phases of the transition are identical. A PT is easily seen on a graph of the spontaneous magnetism versus the temperature of the system as a discontinuity of the data, or a point where the temperature remains constant while the energy input increases [13].

## **2.6 Ising Model**

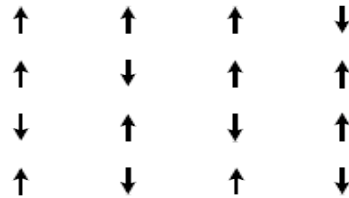
Ising model is a mathematical model of FM in statistical mechanics, which was invented by Wilhelm Lenz (1920). Wilhelm Lenz gave the model as a problem to his student Ernst Ising. Ising solved this problem in one-dimension in his PHD thesis (1924), which worked on linear chains of coupled magnetic moments. Rudolf Peierls named this model by Ising model in his 1936 publication “On Ising’s model of ferromagnetism”. Lars Onsager,

winner of the 1968 Nobel Prize in Chemistry, solved two dimensional Ising model in 1944 and exhibited phase transition. And then Ising model enjoyed increased popularity and took its place as the preferred basic theory of all cooperative phenomena [14].

A simple classical approximation to an atomic or electronic magnetic moment is provided by an Ising spin which can take two values

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

A two-dimensional magnet can be modeled by a set of  $N_S$  spins located on a fixed two-dimensional lattice of sites. For example, we can have a square lattice with  $L$  spins in the  $x$  direction and  $L$  in the  $y$  direction such that  $L^2 = N_S$  as shown in figure.2.2, the up and down arrows represent a positive and negative spin respectively [15].



**Figure 2.2 Two Dimensional Lattice of Ising Model**

The model we will employ in studies of phase transitions (PT) at finite temperature for magnetic systems its simplest form the Hamiltonian is expressed as:

$$H = -J \sum_{\langle i,j \rangle} S_i S_j - B \sum_i S_i \quad (2.4)$$

with  $S_i = \pm 1$ ,  $J$  is a coupling constant expressing the strength of the interaction between neighboring spins and  $B$  is an external magnetic field interacting with the magnetic moment set up by the spins. The symbol

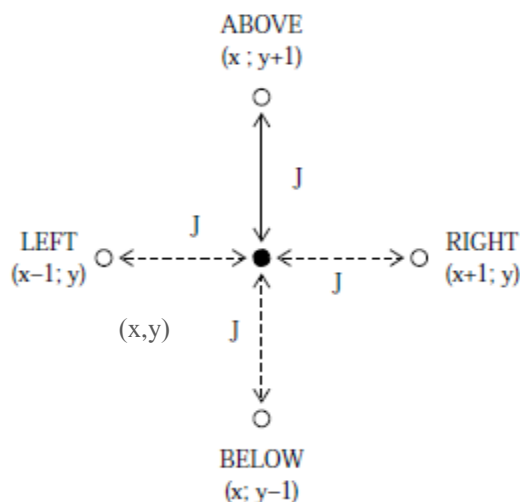
$\langle ij \rangle$  indicates that we sum over nearest neighbors only. If the interaction strength  $J > 0$  the system is ferromagnetic: the energy is minimized if the spin point in the same direction  $S_i S_j = +1$ . If  $J < 0$  the system is antiferromagnetic.  $B$  represents an external magnetic field which couples to the magnetization [15].

Periodic boundary conditions are assumed so that each spin  $S_{i,j}$  has four nearest neighbors  $S_{i+1,j}$ ,  $S_{i-1,j}$ ,  $S_{i,j+1}$  and  $S_{i,j-1}$ . Each spin interacts with these four nearest neighbors (as shown in figure 2.3, the dark dot at position  $(x,y)$ , is being interacted upon by its neighbors which are in one lattice spacing from it.) so that it has a potential energy given by

$$E_{i,j} = -JS_{i,j} \{S_{i+1,j} + S_{i-1,j} + S_{i,j+1} + S_{i,j-1}\} \quad (2.5)$$

The change in energy  $\Delta E$  due to flip of the spin can simply be [15]

$$\Delta E = 2JS_{i,j} \{S_{i+1,j} + S_{i-1,j} + S_{i,j+1} + S_{i,j-1}\} \quad (2.6)$$



**Figure 2.3 Nearest Neighbor Coupling Spin**

## 2.7 Monte Carlo(MC) Method

Monte Carlo (MC) simulations involve generating a subset of configurations or samples, chosen using a random algorithm from a configuration space, according to a probability distribution or weight function. Observables are then computed as averages over the samples.

$$S_1 = +1; S_2 = -1; S_3 = +1, \dots, S_N = +1 \quad (2.7)$$

In which each spin is set up or down. According to statistical mechanics, the average value of an observable is got by weighting each configuration with the Boltzmann factor. For example, the average magnetization at some fixed temperature T is given by

$$\langle M \rangle = \frac{\sum_{all\ states} M e^{-E/K_B T}}{\sum_{all\ states} e^{-E/K_B T}} \quad (2.8)$$

Probability Distribution or weight function is the basic idea of a Monte Carlo (MC) calculation random. The Boltzmann factor is an is to generate a reasonable number of configurations at exponential function of energy which can vary enormously. The random configurations are therefore generated with probability determined by this exponential factor [16].

$$P(S_1, S_2, \dots, S_{N_S}) = \frac{e^{-E(S_1, S_2, \dots, S_{N_S}) / K_B T}}{\sum e^{-E/K_B T}} \quad (2.9)$$

## 2.8 Metropolis Algorithm(MA)

The algorithm of choice for solving the Ising model is the approach proposed by Metropolis et al in 1953. New configurations are generated from a previous state using a transition probability which depends on the energy difference between the initial and final states.

The probability of the nth state for finding the system in a state n is given by

$$P_n(t) = e^{-E_n / K_B T} / Z \quad (2.10)$$



With energy  $E_n$  and  $Z$  is a normalization constant which defines the partition function. In the canonical ensemble.

$$Z = \sum_n e^{-E_n/K_B T} \quad (2.11)$$

It is difficult to compute since we need all states. In a calculation of the Ising model in two dimensions, the number of configurations is given by  $2^N$  with  $N = L \times L$  the number of spins for a lattice of length  $L$ . Fortunately, the Metropolis algorithm considers only ratios between probabilities and we do not need to compute the partition function at all.

The algorithm in step form goes as follows:

1. Fix the temperature.
2. Establish an initial state with energy  $E_b$  by positioning yourself at a random configuration in the lattice.
3. Change the initial configuration by flipping e.g., one spin only. Compute the energy of this trial state  $E_t$ .
4. Calculate  $\Delta E = E_t - E_b$ . The numbers of values  $\Delta E$  is limited to five for the Ising model in two dimensions see the discussion below.
5. If  $\Delta E \leq 0$  we accept the new configuration, meaning that the energy is lowered and we are hopefully moving towards the energy minimum at a given temperature. Go to step 8.
6. If  $\Delta E > 0$ , calculate  $w = e^{-(\Delta E/K_B T)}$ .
7. Compare  $w$  with a random number  $r$ ;  $r$  in  $[0,1]$ . If

$$r \leq w$$

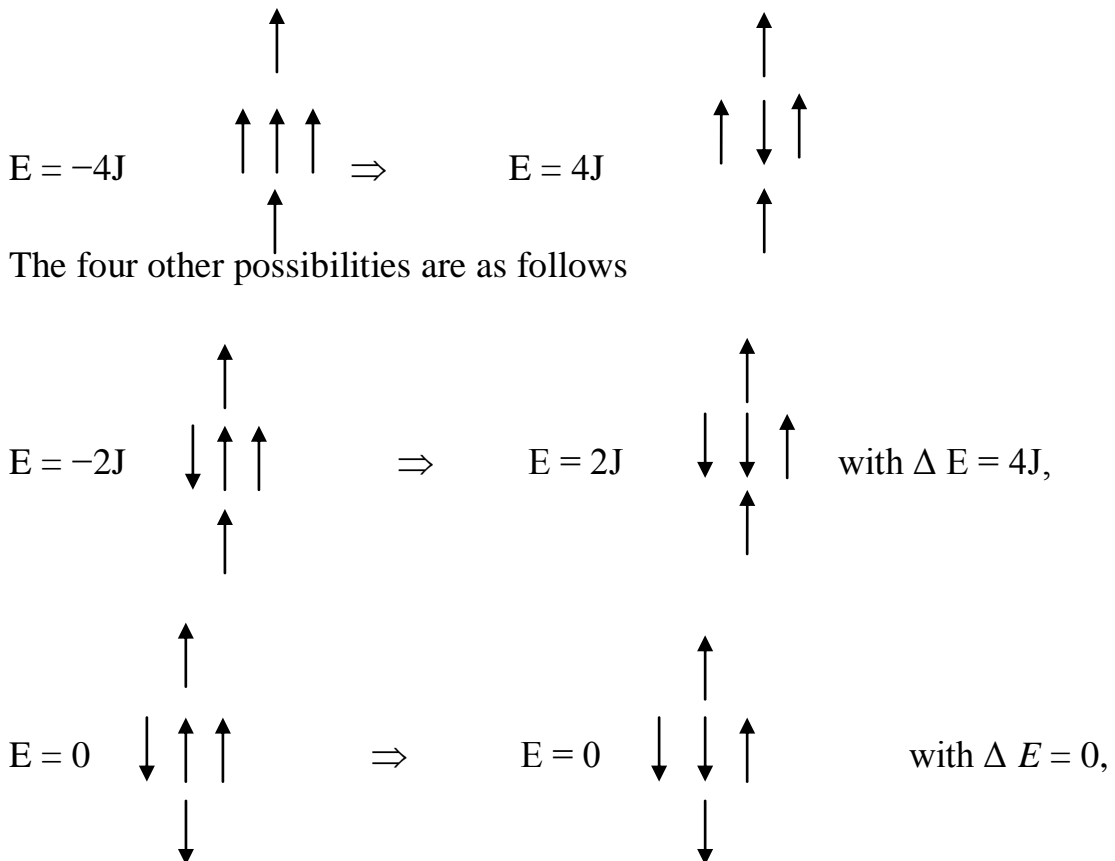
then accept the new configuration, else we keep the old configuration.

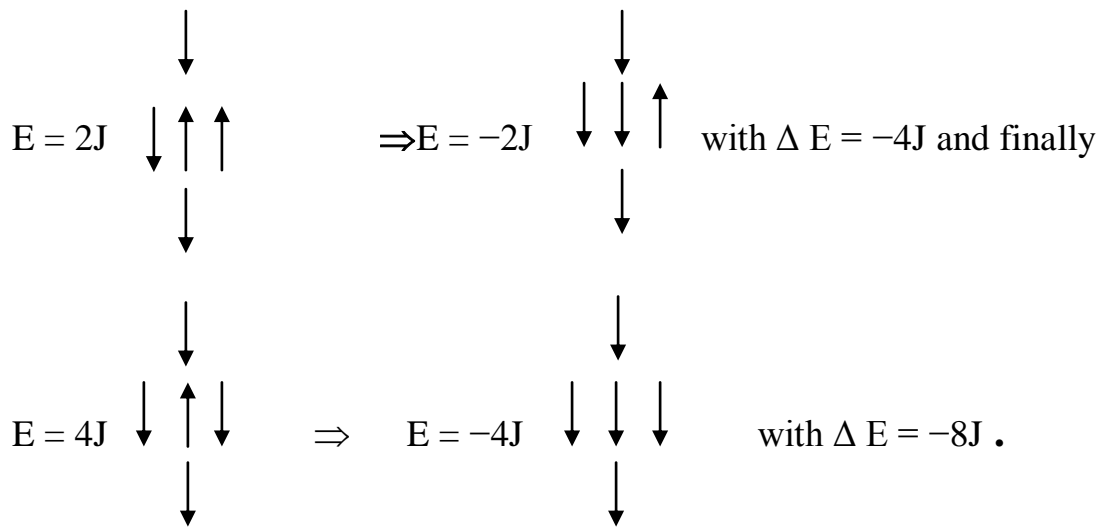
8. The next step is to update various expectations values.
9. The steps (3)-(8) are then repeated in order to obtain a sufficiently good representation of states.
10. Each time you sweep through the lattice, i.e., when you have summed over all spins, constitutes what is called a Monte Carlo cycle. You could think of one such cycle as a measurement. At the end, you should divide the various expectation values with the total number of

cycles. You can choose whether you wish to divide by the number of spins or not. If you divide with the number of spins as well, your result for e.g., the energy is now the energy per spin.

The crucial step is the calculation of the energy difference and the change in magnetization. This part needs to be coded in an as efficient as possible way since the change in energy is computed many times. In the calculation of the energy difference from one spin configuration to the other, we will limit the change to the flipping of one spin only. For the Ising model in two dimensions it means that there will only be a limited set of values for  $\Delta E$ .

Actually, there are only five possible values. To see this, select first a random spin position  $x,y$  and assume that this spin and its nearest neighbors are all pointing up. The energy for this configuration is  $E = -4J$ . Now we flip this spin as shown below. The energy of the new configuration is  $E = 4J$ , yielding  $\Delta E = 8J$  [12].

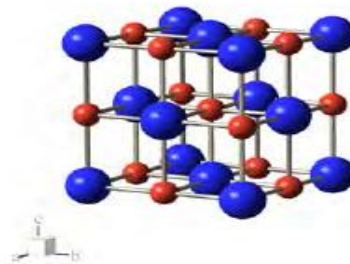




## 2.9 Nickel Oxide(NiO) Structure

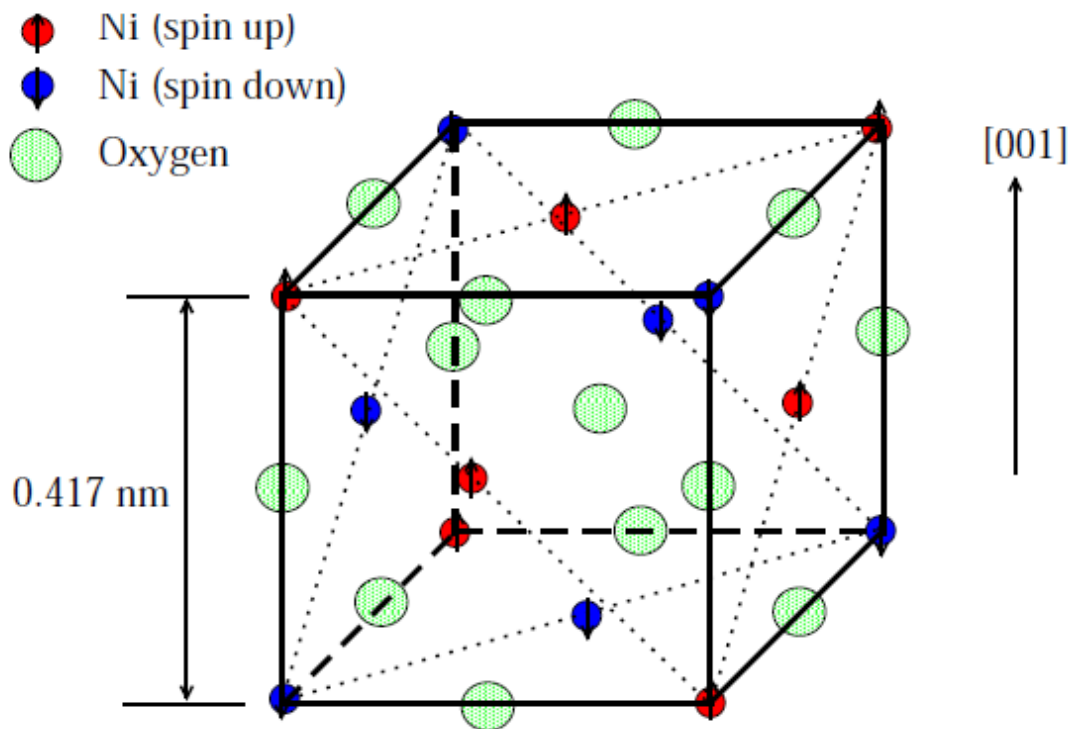
Nickel oxide( NiO) also known as bunsenite after R. Bunsen, was discovered in 1858 and is only found pure in nature in a few locations around the world. The bulk mineral has a deep green color while nanoparticles of NiO are black [17].

Bulk NiO has a face centered cubic (fcc) NaCl structure with the space group Fm3m, and a lattice parameter of  $a = 4.177 \text{ \AA}$  (see figure 2.4). There are two components of spin configurations due to the non-local exchange interaction. For the first component, the direct exchange interaction between the nearest neighbor of Ni ions favors pairing of spins to lower energy. For another one, a very strong interaction comes from the super exchange between the next-nearest neighbor of Ni ions. This makes the antiferromagnetic spin structure for the ground state of NiO [18], this cubic structure is illustrated in Figure 2.4.



**Figure 2.4 Cubic Crystal Structure of NiO. Ni is Shown as Blue and Oxygen as Red.**

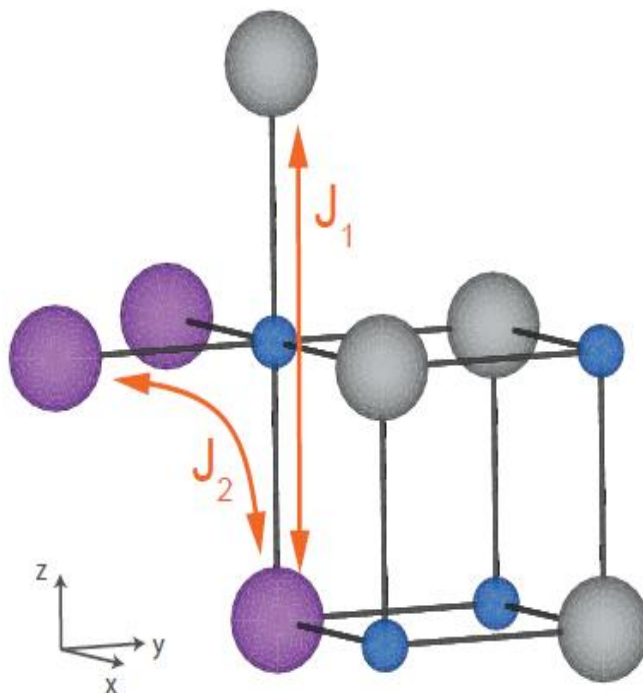
NiO is a type-II antiferromagnet (AF) with an antiferromagnetic ordering vector of  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ , i.e. along the space diagonal of the unit cube and the spins confined to the (111) plane. Below the N'eel temperature of 523 K there is a slight contraction of the cubic structure along the [111] direction, known as exchange striction. However, this contraction is less than 0.3% in bulk NiO and it will not be considered, also it is paramagnetic above that temperature [17].



**Figure 2.5 Structure of NiO Showing the Antiferromagnetic (AF2) Spin Structure**

NiO is one of the typical systems on which different calculation schemes are tested. It is a charge-transfer insulator with a band gap  $\sim 4$  eV and local magnetic moment of  $1.77\mu_B$ . This type of magnetic ordering is due to the strong next-nearest-neighbor (nnn) coupling between nickel ions via oxygens 2p shell. The N'eel temperature is  $NT = 523$  K.

First of all, the dominating exchange interactions between second nearest neighbors was calculated,  $J_1$  (see Figure. 2.6), using conventional total energy technique and obtained  $J_1 = 18.8$  meV, which agrees extremely well with experimental estimation of  $J_1 = 19.0$  meV. The exchange constants calculated by the Green's function method are  $J_1 = 18.9$  meV, and  $J_2 = -0.4$  meV, and agree with both the total energy and experimental estimations [19].



**Figure 2.6 Schematic View of the NiO Crystal Structure. The Blue Spheres Denote Oxygen Ions, While the Gray And Magenta Spheres Denote Two Magnetic Types of Ni**

# Chapter Three

## Simulation Process

### 3.1 Introduction

There are many possible approaches to study the effect of temperature on Nickel Oxide (NiO) structure. This chapter uses a simulation approach to investigate and verify the phase transition (PT) of (NiO).

To analyze the effect of temperature changes on NiO structure through analysis of NiO's phase transition, the work was split into the following distinct parts:

- A flow chart was designed for the simulation process.
- The simulation process was verified by converting the designed flow chart to a computer program.

The proposed work to simulate the effect of temperature on NiO structure by using a computer program to analyze the phase transition.

The Ising model, Monte Carlo (MC) method and Metropolis algorithm(MA) which were used for Statistical mathematical, numerical method and the simulation's steps respectively were used to show this work.

A computer with Ubuntu Linux operating system will be used in a simulation environment for implementing the simulation program, and the simulated results using C<sup>++</sup> will be used to evaluate the proposed work.

The first and most compelling reason for using C<sup>++</sup> is because it is fast, with careful programming and optimizations; also it can be compiled to a machine code program which is able to use the full power of the available hardware. A second reason for using C<sup>++</sup> is that there is a wealth of numerical libraries for scientific computing in C<sup>++</sup> and related languages. Moreover it has a flexible memory management model. A final reason to program in C<sup>++</sup> is that it is an

object-oriented language. It is widely held that writing in an object-oriented style leads to programs which are easier to understand, to extend, to maintain and to refactor [20].

### 3.2 Simulation Procedure

The two dimensional (2D) square lattice of spins was considered in this work. In the absence of external magnetic field, the Hamiltonian of a spins system is written as:

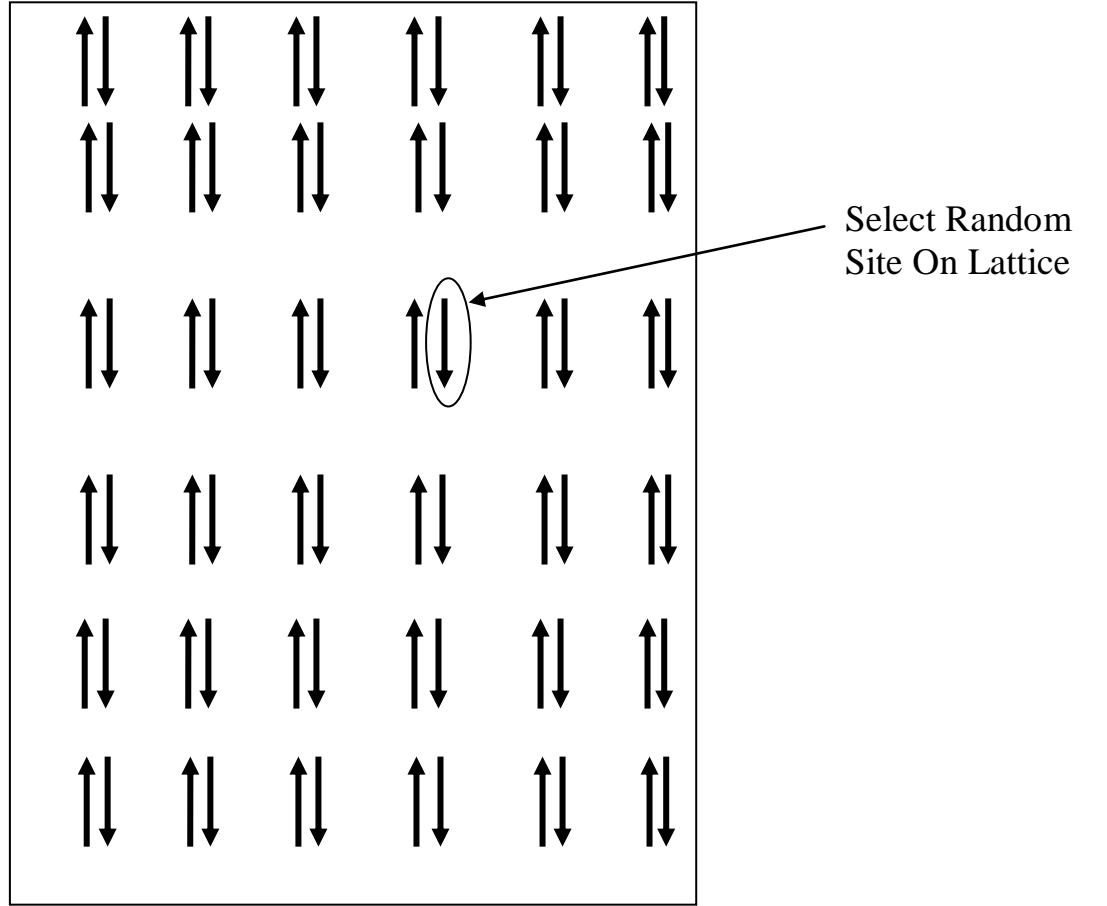
$$H = -J \sum_{(i,j)} S_i S_j \quad (3.1)$$

Where  $J$  is the interaction energy of the two spins,  $N$  is the total number of spins and  $S_i$  and  $S_j$  are the spin along x and y direction respectively.

The temperature ( $T$ ) was fixed and then was increased gradually from absolute zero. And at critical temperature  $T_c$ , the magnetization changes its state from high value to low value (this is when phase transition occurs).

A Monte Carlo (MC) simulation for 6 x 6 square lattice (SL) of NiO (as represent in figure 3.1) has been implemented, and from various diagrams the critical temperature ( $T_c$ ), energy ( $E$ ), magnetism ( $M$ ), specific heat ( $C_v$ ) and magnetic susceptibility ( $\chi$ ) were determined for the square lattice used.

Here it has been assumed that only the nearest neighbors affect each spin (that is, in a two dimension (2D) SL, each spin has four neighbors, up, down, left and right).



**Figure 3.1 6X6 Spin Square Lattice**

The observables or thermodynamic quantities which were determined in the simulation are energy (E), magnetization ( M), energy average $\langle E \rangle$ , average of square energy $\langle E^2 \rangle$ , magnetization average $\langle M \rangle$  and average of square magnetization $\langle M^2 \rangle$ .

The magnetization (M) per spin in a state n was given by

$$M_n = \sum_{i=1}^N S_i^n \quad (3.2)$$

Since only one spin k flips at a time in the Metropolis algorithm, so the change in magnetization was given by

$$\Delta M = M_m - M_n = \sum_{i=1}^N S_i^m - \sum_{i=1}^N S_i^n = S_k^m - S_k^n = 2S_k^m ; S_k^n = -S_k^m \quad (3.3)$$

The magnetization average  $\langle M \rangle$  and energy average were given as follows:

$$\langle M \rangle = \frac{1}{N_2} \sum_i^{N_2} M(S_i) \quad (3.4)$$



$$\langle E \rangle = \frac{1}{N_2} \sum_i^{N_2} E(S_i) \quad (3.5)$$

Where  $N_2$  is the size of the lattice  $N_2 = 6 \times 6$ .

Using the Hamiltonian in equation (3.1) the energy (E) is determined as shown below:

$$E = \sum_i^N H_i = -J \sum_i^N s_i s_j \quad (3.6)$$

$$E_{i,j} = -\{J_1 S_{i,j} \{S_{i+1,j} + S_{i-1,j} + S_{i,j+1} + S_{i,j-1}\} + J_2 S_{i,j} \{S_{i+1,j} + S_{i-1,j} + S_{i,j+1} + S_{i,j-1}\}\} \quad (3.7)$$

Where  $J_1$  and  $J_2$  were the exchange interaction for the NiO and their values are 19.0 meV and -0.4 meV respectively[19 ].

The change in energy  $\Delta E$  due to flip of the spin can simply be

$$\Delta E = 2J_1 S_{i,j} \{S_{i+1,j} + S_{i-1,j} + S_{i,j+1} + S_{i,j-1}\} + 2J_2 S_{i,j} \{S_{i+1,j} + S_{i-1,j} + S_{i,j+1} + S_{i,j-1}\} \quad (3.8)$$

For every spin the specific heat ( $C_V$ ) and the susceptibility ( $\chi$ ) were calculated as follows:

$$C_V = \frac{\partial E}{\partial T} = \frac{(\Delta E)^2}{K_B T} = \frac{\langle E^2 \rangle - \langle E \rangle^2}{K_B T^2} \quad (3.9)$$

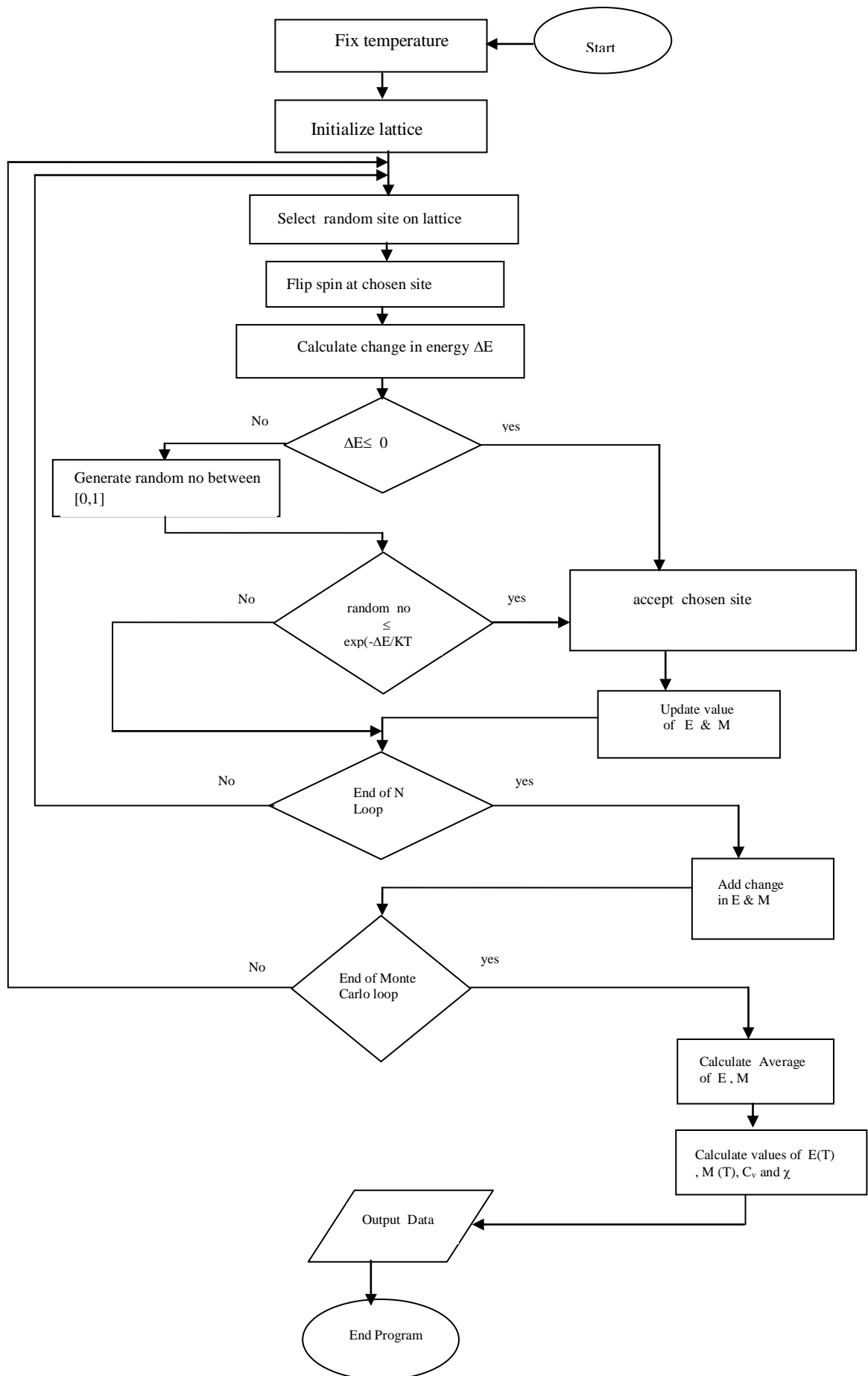
$$\chi = \frac{\partial M}{\partial T} = \frac{(\Delta M)^2}{K_B T} = \frac{\langle M^2 \rangle - \langle M \rangle^2}{K_B T} \quad (3.10)$$

### 3.2.1 Design an Algorithm

As stated before that MA is choice for solving the Ising model and it was presented in details in chapter two section 2.8.

### 3.2.2 Simulation Flow Chart

The steps executed in the program were summarized in a flowchart (see Figure 3.2) to show what the algorithm is designed to achieve.



**Figure 3.2 Simulation Flow Chart**

# Chapter Four

## Results and Discussion

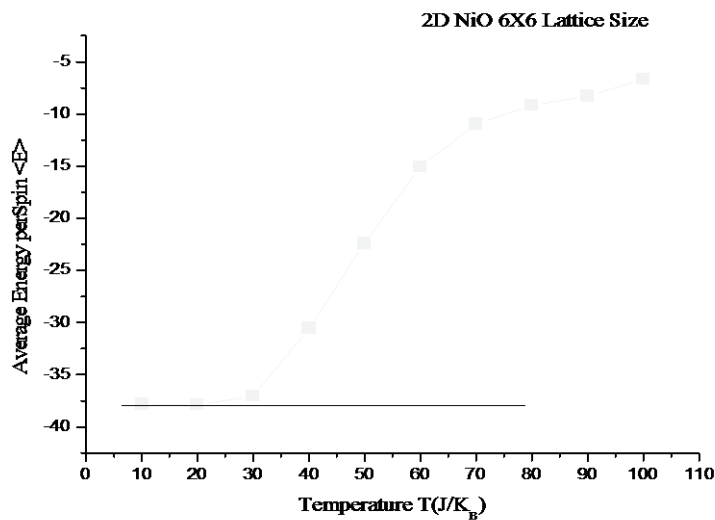
### 4.1 Introduction

This chapter includes a discussion of results for the effect of temperature on magnetization (M), specific heat  $C_v$  and magnetic susceptibility  $\chi$  of 2D NiO for 6X6 SL, also it presents thesis conclusion and recommendations.

### 4.2 Results and Discussion

#### 4.2.1 Effect of Temperature on Average Energy of NiO

The graph in (Figure. 4.1) depicts the average energy was plotted as a function of temperature of NiO square lattice (SL), it is noted that the average energy increases when the temperature increases and from this the ground state was determined to be  $-38.125$  meV. The value of ground state was very close to the result observed by Danny Bennett  $-36.75 \pm 0.01$  meV [7].

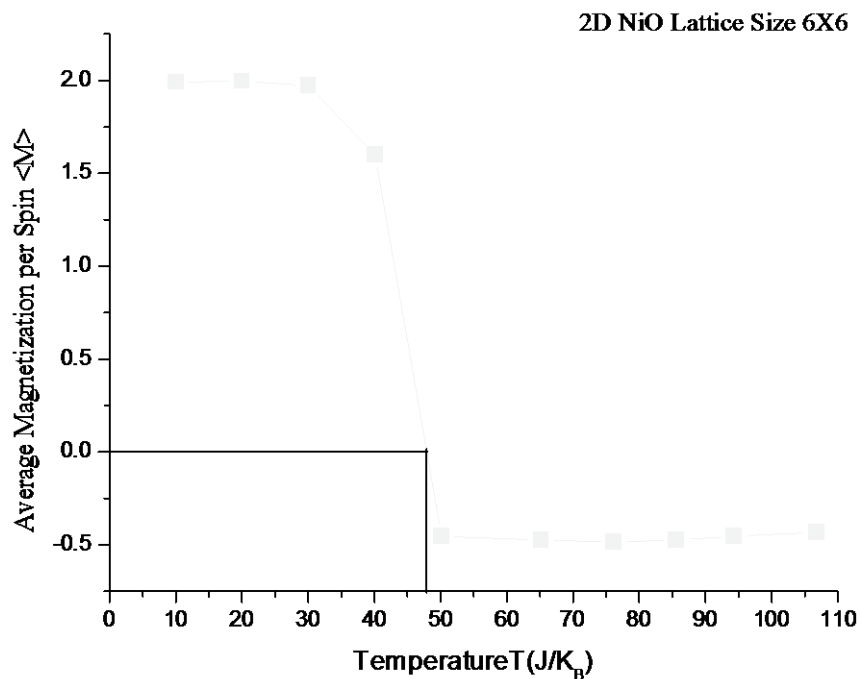


**Figure 4.1. plot of average energy against temperature T for 6x6 square lattice of NiO**

## 4.2.2 Effect of Temperature on Average Magnetization of NiO

Figure 4.2. elucidates the relationship between average magnetization per spin and temperature, it is observed that the magnetization is maximum at low temperatures (ordered state) and vanishes at high temperatures, also the magnetization values decreases from positive to negative value, this points to the fact that the phase transition occurred at the critical temperature  $T_c \approx 47.2679045 \text{ J/K}_B$  and the NiO translated from antiferromagnetic to a diamagnetic state.

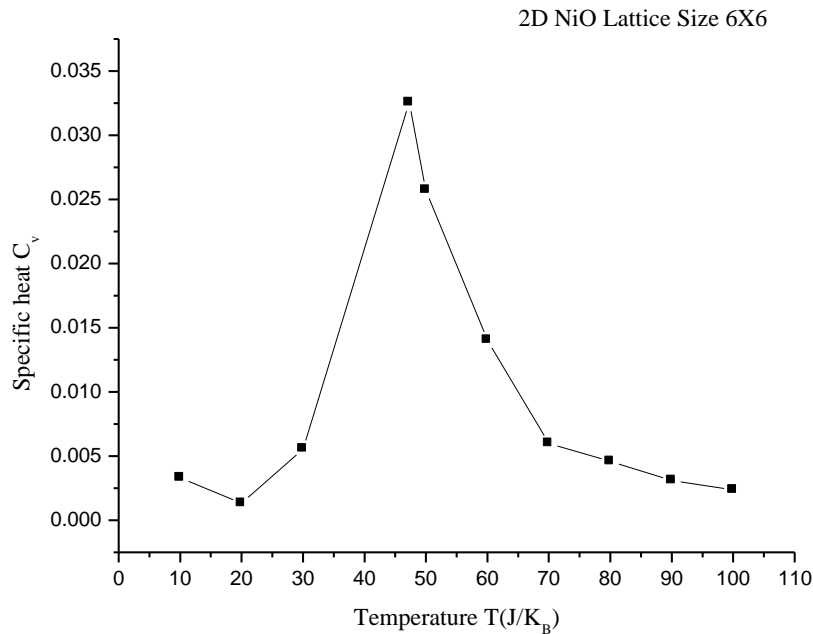
This result shows a different behavior compared to the results observed by Danny Bennett [7], the difference may be attributed to difference values for exchange interaction and temperature range of NiO ( $J_1=19$  and  $J_2 = -0.4$ , temperature range from 10 to 100 in units of  $\text{J/K}_B$ ), while Danny Bennett was took  $J_1 = 2.3$  and  $J_2 = -21$  and low temperature range from 1 to 5.



**Figure 4.2.**A plot of average magnetization per spin vs temperature of 2D NiO for 6X6 square lattice

### 4.2.3 Effect of Temperature on Specific Heat of NiO

From figure 4.3 it clear that when temperature increases the NiO was transited from antiferromagnetic state to diamagnetic state due to change in specific heat which was observed at critical temperature  $T_c \approx 47.2679045$  J/K<sub>B</sub>. This is in accordance with what has been observed in the graphs representing the average magnetization(see Fig. 4.2).

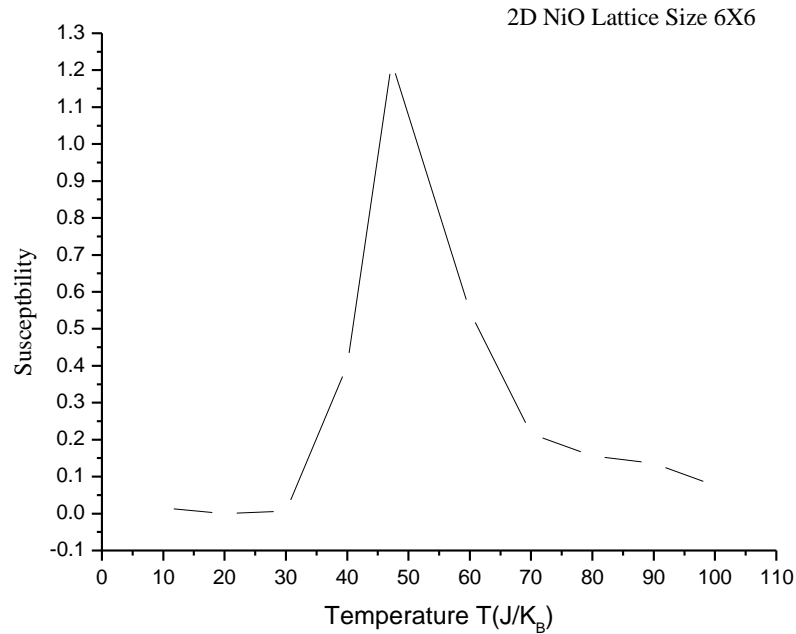


**Figure 4.3 Plot of specific heat  $C_v$  VS temperature  $T$  for 6x6 square lattices of 2D NiO**

### 4.2.4 Effect of Temperature on Magnetic Susceptibility of NiO

Figure 4.4 illustrates that the magnetic susceptibility is minimum at low and high temperature and has a sharp jump and maximum value at the critical temperature  $T_c \approx 47.2679045$  J/K<sub>B</sub>.

This change for magnetic susceptibility due to change of magnetization(see equation ( 3.10) ) and also is in accordance with what has been observed in the graph representing the specific heat(see fig 4.3).



**Figure 4.4. Magnetic susceptibility of a NiO as a function of temperature for 6x6 square lattices.**

### 4.3 Conclusion

The simulation have started with random spin at the lattice sites and calculated initial magnetization and energy using Ising model. And Metropolis Monte Carlo simulation of an Ising model in C++ was implemented. All the simulations were of 6 x 6 square lattices of NiO, the temperature was run from 10 J/K<sub>B</sub> to 100 J/K<sub>B</sub>. After each temperature increment, the system was allowed to equilibrate. The material was described by 2D square lattice having nearest and second nearest neighbor interactions with interaction energies of  $J_1 = 19$  and  $J_2 = -0.4$ , respectively. As the oxygen atoms have no magnetic moment, then it was ignored only the nickel atoms were considered, and the Boltzmann's constant was set to  $K_B = 1$ . The simulation code is shown in appendix A.

2D Ising model of NiO was investigated and developed Successfully. By plotting the graphs of some thermodynamic functions describing the system such as average energy, average magnetization and specific heat, magnetic

susceptibility which were conclude that the system undergoes a phase transition from an antiferromagnetic state to a diamagnetic state at critical temperature  $T_c \approx 47.2679045 \text{ J/K}_B$ .

However, The ground state was determined to be  $-38.125 \text{ meV}$  which is very close to the result observed by authors.

#### **4.4 Recommendations**

For more study, further research will be needed in many areas, including:

- The simulation was implemented for 6X6 lattice size and temperature range of 10 to 100  $\text{J/K}_B$ , further work would be done on a larger system lattice size, a smaller temperature step and a larger number of averaged simulations.
- Future work can be done in simulation using other programming languages such as Java, Fortran and Python and etc.
- Finally, since this simulation was applied on NiO using 2D Ising model, the simulation can be extended to higher dimension of Ising model (i.e. 3D Ising model) or using other models such as Heisenberg model, XY model and etc.

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# Appendix A

## The Simulation Program

```
#include <iostream>
#include <cmath>
#include <ctime>
#include <random>
#include <fstream>

using namespace std;

const int Nx = 6; //Spins in direction x
const int Ny = 6; // Spins in direction y
const int N2 = Nx*Ny; // all Spins
int MCSteps = 2^N2; // number of Metropolis Steps
const int k_B = 1; // Boltzmann constant
const int B = 0; //magnetic field
const int J = -1; // antiferromagnetic coupling
const int mu = 1; //permeability
const int J1 = 19; //first energy exchange interaction of Ni
const int J2 = -0.4 ;// second energy exchange interaction of Ni
double beta; // inverse temperature
double T; // temperature
int s[Nx][Ny]; //spin
int li[N2] , lj[N2] , ri[N2] , rj[N2]; //spin neighbors
int i; //spin position in direction x
int j; // spin position in direction y
double dE; // energy difference (E_new - E_old)
double E; // energy
double Cv; //specific heat
//double a_Cv; // analytical results specific heat
double sus; // susceptibility
//double a_sus; // analytical results susceptibility
double tprob; // transmission probability
double rprob; // random probability between 0 and 1
double mag; // magnetization
double med_mag; // mean magnetization
double med_mag2; // mean squared magnetization
double med_E; // mean energy
double med_E2; //mean squared energy
int count1; //counter
```

```

int count2; //counter
//beta = 1/(k_B*T);

//generates an initial spin
//configuration randomly spin up (+1) spin down (-1)
void Initialisierung () //initialization

// random start +1 order -1

{
random_device seed;
mt19937 engine(seed());
uniform_real_distribution<double> values(0.0, 1.0 );
for(int i=0; i<Nx; ++i)
for(int j=0; j<Ny; ++j)
{
if(values(engine)<0.5) { s[i][j] = 1;}
else { s[i][j] = -1;}
}

//cout<<"starting position:"<<s[i][j]<<"\n";

}

// measurement of the magnetization
double Magnetisierung() // magnetization
{
int Magnetisierung = 0;
for(int i =0; i<Nx; i++)
for(int j=0; j<Ny; j++)
{
Magnetisierung += s[i][j];
}
return Magnetisierung;
}

//measurement of the energy
double Energie() // energy
{

int sumN =0;

```

```

for(int i=0; i<Nx; i++)
for(int j=0; j<Ny; j++)
{
mag += s[i][j];
int ri = i == Nx-1 ? 0 : i+1;
int rj = j == Ny-1 ? 0 : j+1;
sumN += s[i][j] * (s[ri][j] + s[i][rj]);

}
return -(J1*sumN + J2*sumN)+mu*B*mag;
}
//One of N2 spins is choosen randomly
//defines next neighbours
//implement periodic boundarys
//makes one metropolis step
void OneMetropolisStep()
{
random_device seed;
mt19937 engine(seed());
uniform_int_distribution<int> value1(0, Nx);
int i = value1(engine);
uniform_int_distribution<int> value2(0, Ny);
//cout <<"i:"<<i<<"\n";
int j = value2(engine);
//cout<<"j:"<<j<<"\n";

// nearest neighbours
int li;
if(i==0)
li = Nx-1;
else
li = i-1;

int ri;
if(i == Nx-1)
ri = 0;
else
ri = i+1;

int lj;
if(j==0)
lj= Ny-1;
else

```

```

lj = j-1;

int rj;
if(j == Ny-1)
rj = 0;
else rj = j+1;

mag = Magnetisierung();
E = Energie();

//mag= N2*s[i][j];
//E=-J1*(s[i][ri]*s[j][rj]) - J2*(s[i][ri]*s[j][rj])+mu*B*mag ;

beta=1/(k_B*T);

dE = 2*J1*s[i][j]*(s[ri][j] + s[li][j] + s[i][rj] + s[i][lj]) +
2*J2*s[i][j]*(s[ri][j] + s[li][j] + s[i][rj] + s[i][lj])+2*mu*B*s[i][j];

if(dE<=0)

{
s[i][j]=-s[i][j];

mag= mag+2*s[i][j];
E=E+dE;
}
else
{
random_device seed;
mt19937 engine(seed());
uniform_real_distribution<double> values(0.0, 1.0 );
tprob=exp(-beta*dE);
rprob= values(engine);
if (rprob<=tprob)
{
s[i][j]=-s[i][j];

mag=mag+2*s[i][j];
E=E+dE;
}
else
{
s[i][j]=s[i][j];
mag = mag;
E=E;
}
}

```

```

}

}

}

// N2 Metropolis Steps
// magnetisation per spin
// energy per spin
void oneMetropolisStepPerSpin()
{
for (int i =0; i<N2; i++)
{
OneMetropolisStep()

}
mag = mag / N2;
E = E / N2;

}

int main( )
{

for(count1=0; count1<MCSteps; count1++)
{
Initialisierung();
}
//T=10;
for (T=10; T<=100; T+=10)
{
cout << " Temperatur: " << "\t"<<T << "\t";
beta = 1/(k_B*T);

med_mag =0;
med_E =0;
med_mag2 =0;
med_E2 =0;

```

```

int MM = int(0.2* MCSteps); //perform thermalization steps to let the
system come to equilibrium
for(int count1=0; count1< MM; count1++)
{
oneMetropolisStepPerSpin();

med_mag += mag;
med_mag2 += mag*mag;
med_E+= E;
med_E2 += E*E;

}

med_mag=med_mag/(MM);
med_mag2=med_mag2/(MM);
med_E=med_E/(MM);
med_E2=med_E2/(MM);

Cv=(med_E2-med_E*med_E)/(T*T); //specific heat
sus=N2*(med_mag2-med_mag*med_mag)/(T); // susceptibility

// analytical solution:
//a_Cv = (k_B* pow(beta, 2)* pow(J,2))/(pow(cosh(beta * J),2));
//a_sus = beta*exp(2*beta*J);

//cout <<" magnetization " <<"\t"<<mag<<"\t";
//cout <<" energy: " <<"\t"<<E<<"\t";

cout <<"mean magnetization " <<"\t"<<med_mag<<"\t";
cout <<"mean energy: " <<"\t"<<med_E<<"\t";
//cout <<"mean squared magnetization : " <<"\t"<<med_mag2<<"\t";
//cout <<"mean squared energy: " <<"\t"<<med_E2<<"\t";
cout <<"specific heat: " <<"\t"<<Cv<<"\t";
//cout <<"analytical Cv:" <<"\t"<<a_Cv<<"\n";
cout <<"susceptibility : " <<sus<<"\n";
//cout <<"analytical sus: " <<a_sus<<"\n";

}

return 0;

}

```



## List of Abbreviations

<b>Abbreviation</b>	<b>Meaning</b>
2D	Two Dimension(al)
AF	Antiferromagnetic /Antiferromagnetism
DM	Diamagnetic / Diamagnetism
FCC	Face Centered Cubic
FM	Ferromagnetic / Ferromagnetism
MA	Metropolis Algorithm
MC	Monte Carlo
Ni	Nickel
NiO	Nickel Oxide
PM	Paramagnetic / Paramagnetism
PT	Phase Transition
SL	Square Lattice
TC	Curie Temperature
NT	Neel Temperature