MAGNETIC FIELD EFFECT OF SPIN DISTRIBUTION IN FERROMAGNETIC MATERIALS USING MONTE CARLO SIMULATION OF TWO - DIMENSIONAL ISING MODEL

BY

DAVID, MARGARET JOHN

DEPARTMENT OF PHYSICS, FACULTY OF SCIENCE,
AHMADU BELLO UNIVERSITY, ZARIA
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DAVID, MARGARET JOHN

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DECLARATION

I **David Margaret, John** hereby declare that the work in this Thesis entitled "**Magnetic Field Effect of Spin Distribution in Ferromagnetic Material Using Monte Carlo Simulation of 2 – D Ising Model"** has been performed by me in the department of Physics under the supervision of Prof. I.O B Ewa and Dr. P.O Akusu.

Information derived from other literature works has been duly acknowledged in the text and a list of references provided. No part of this work was previously presented for another degree or diploma at any university or institution.

Margaret, John David **Date**

CERTIFICATION

This Thesis entitled "**Magnetic Field Effect of Spin Distribution in Ferromagnetic Material Using Monte Carlo Simulation of Two – Dimensional Ising Model"** by Margaret, John David meets the regulations governing the award of the degree of Masters of Science of Ahmadu Bello University, and is approved for its contribution to scientific knowledge and literary presentation.

(Chairman, Supervisory Committee)	**Date**
(Prof. I.O.B Ewa)	
(Member, Supervisory Committee)	**Date**
(Dr. P.O Akusu)	
(Head of Physics Department)	**Date**
(Dr. U. Sadiq)	
(Dean, Postgraduate School)	**Date**
(Prof. A. A. Joshua)	

DEDICATION

This work is dedicated to God Almighty who has been my helper and protector throughout this period of study and to my Entire family members.

ACKNOWLEDGEMENTS

I give all glory to Almighty God for sparing my life to enable me complete this program upon the challenges faced. The Horse is prepared for the days of Battle but safety is of the Lord.

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ABSTRACT

This work discussed the 2 - D Ising Model as a magnetic model in an applied magnetic field under a range of Thermalization sweep. The Monte Carlo Simulation produces the effect of magnetic properties on spin distribution of a ferromagnetic coupling. The essence is to accurately determine the behavior of the two spin state under magnetic influence in consideration of spin energy, spin magnetization, susceptibility and specific heat.The simulation validates the known result obtained by a rigorous statistical computation which reduces free energy of the system and approximated the values of the coefficient for partition function.The low-temperature series expansion for the partition function of the two-dimensional Ising model was determined exactly for finite lattices using Monte Carlo Simulation. The exact distribution function for the energy with its respective magnetization and specific heat was also determined from the coefficients of the partition function. This provides an exact solution with which one can compare energy histograms determined by the Onsager's solution. This solution will be useful for detailed studies of statistical and systematic errors in histogram reweighting.

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CHAPTER ONE

1.0 INTRODUCTION

The Magnetic field is a force field created by the motion of an electric charge due to electric field that vary in time, and by the intrinsic magnetic moment of elementary particles associated with the spin of the particle. The flow of electrical current in a wire (macroscopic) produces magnetic field, so also the motion of electrons around a nucleus of an atom (microscopic) produces a magnetic field associated with an individual atom. Magnetic field at any given point is specified by both direction and magnitude (strength) which qualifies it as a vector field. The atomic magnets produced are like ordinary magnetic vectors having north and South poles pointing in random directions. By so doing the magnetic fields from individual atoms cancels out giving zero resultant magnetic field (occurs in any macroscopic clump of matter).

The implication of these is that the ions are completely anti-aligned and this normally happens at a temperature lower than a characteristic temperature known as the Curie temperature (Huang,1992). However, in some ferromagnetic material, it is possible for a very large numbers to line up giving a non-zero total magnetic field, Iron (Fe) and Nickel (Ni) are very good example of such material.

Similarly, an electron has a magnetic field from its intrinsic magnetic moment due to both its charge and its intrinsic spin. The spin of an electron combined with its electric charge, results in a magnetic dipole moment and creates a magnetic field. Although an electron can be visualized classically as a spinning ball of charge, spin is a quantum mechanical property with differences from the classical picture, due to the fact that it is

quantized into discrete up/down states. This consequently explains magnetization within an atom. Spin is connected more with its magnetic behavior rather than rotation of an electron about its own axis (Beise, 2002).

However spin being an intrinsic property of a charge particle, has a characteristic quantum number of ½ for a particular particle. In the case of ferromagnetic material, the electrons of its atom obeys the Pauli exclusive principle that stipulates that no two identical particles with half-integer spin should occupy the same quantum state simultaneously, therefore electron spin "up" (clockwise) and "down" (anticlockwise) which create room for two electrons for each set of spatial quantum number, resulting to two possibilities for z-component, x-component or y-component which causes an energy splitting because of the magnetic moment of the electron.

While yet a spinning sphere of charge produce a magnetic moment, the magnitude of the magnetic moment obtained cannot be reasonably used to compute the magnetic properties of that electron, This is so because high energy scattering from electrons shows no size of the electron down to a resolution of about 10^{-3} Fermi, and at that size a preposterously high spin rate of some 10^{32} radian/s would be required to match the observed angular momentum (Nave, 2010).

Under high temperature (above the curie temperature) thermal motion or entropy competes with the ferromagnetic tendency for dipoles to align, resulting in ferromagnetic phase transition (a second – order phase transition) which is a continuous phase transition in which ferromagnetism transit to paramagnetism this is characterized by derivatives of free energy which are magnetization, divergent susceptibility, infinite spin correlation length and divergent heat capacity. Studying these derivatives and its applications is better done by the

Ising model in two Dimensions and solving the model by a computer program simulation known as the Monte Carlo Simulation of 2-D Ising Model.

1.1 STATEMENT OF RESEARCH PROBLEMS.

The problem that was examined in this research work is the effects of magnetic field on spin states distribution of an atom provided by discrete connection of variable which interacts in pairs (spins).

This leads to obtaining a qualitative information on magnetization (magnetic dipole moment), magnetic field, energy, specific heat capacity and magnetic susceptibility by watching the spin array during the simulation. These was done within the content of mathematical model in statistical mechanics known as the Ising Model in two dimension, built with the Boltzmann distribution function which deals with the probability of each configuration of spins with inverse temperature. If the energy of each possible state is specified the Boltzmann function will give the probabilities P(S) for the system to be in each of its possible states at specified temperature, as follows:

$$P(S) = \frac{e^{-E(S)/K_B T}}{\sum_A e^{-E(A)/K_B T}} \qquad (1.0)$$

where :

E(S) = energy of the system when it is in state S.

T = absolute temperature of the system (i.e measured in degree Kelvin).

k_B = is a fundamental constant of nature known as Boltzmann's constant.

The sum in the denominator is over all possible state (A) of the system – which ensures that the sum of the probabilities P(S) for all states S is one.

The configuration was generated using the metropolis algorithm which converge on sequences used in Monte Carlo simulation. Therefore the microscopic quantities of interest can be calculated by doing simple probability sums.

1.2 AIM / OBJECTIVES OF RESEARCH

The aim of this Research work is to produce accurate and reasonable result for spin state distribution due to magnetic effect on ferromagnetic system.

The Objectives are to:

(i) Measure the energy, magnetization, specific heat and susceptibility of the system at each step of the routine in order to validate the Onsager exact solution of 2-D Ising model using a simplified form to obtain magnetic field effect produced by spin of an electron (electric charge) and its angular momentum on a spin state of an atom using the Monte Carlo simulation for 2-dimensional Ising model.

(ii) Further establish the direct influence of two effects (spin and Pauli Exclusion Principle) from Quantum mechanics which could not be done by the motion of classical charged particles.

1.3 SCOPE OF RESEARCH WORK

The scope of this study was limited to ferromagnetic system with many atoms containing an unpaired spins and partially filled shells. Because such can experience a net magnetic moment in the absence of an external field and exhibit strong interaction and spontaneous magnetization. So the interest in the thermodynamics quantities of the system which are:

i) Energy

$$E = \sum_{ij} S_{ij} \quad H(S_i) \qquad (1.1)$$

ii) Magnetization

$$M = \sum_{ij} S_{ij} \left(\sum_{i} S_i \right) \qquad (1.2)$$

iii) Susceptibility

$$\chi = \sum_{ij} S_{ij} \left(\sum_{i} S_i \right)^2 - M^2 \qquad (1.3)$$

iv) Specific heat.

$$C_R = \sum_{ij} S_{ij} H^2 S_i - E^2 \qquad (1.4)$$

where S_{ij} is the spin in the two states, $H(S_i)$ is the applied magnetic field.

1.4 JUSTIFICATION OF THE RESEACH

Ferromagnetism is a phenomena in solid state physics which make metals like Fe and Ni behave in such a way that a finite fraction of the spin of their atoms become spontaneously polarized in the same direction giving rise to a macroscopic magnetic field when temperature is lower than the characteristic curie temperatures (Huang, 1966).

Magnetic moment of an electron is associated with its intrinsic spin, but what is the magnetic field due to spin? This is a question that needs an answer and this research work will provide it. The fact is that you cannot give classical magnetic field to that produced by a quantum mechanical particle, which is why the need to use the Quantum Monte Carlo simulation to get the magnetic field effect of spin distribution of these materials.

There are various significance of this work to field of knowledge and that includes :

1. It produces a simpler and less complicated form of calculating the magnetic properties of a real atom (say iron for instance), which the Boltzmann

probability function in its simplicity could not achieve, due to the fact that an individual atom has a lot of electrons and any macroscopic piece of ferromagnetic material contain an enormous number of individual atoms.

2. It validate or rather authenticate the various application of spin magnetic moment which creates the basis for modern standard model used today in the applications of Nuclear Magnetic Resonance (NMR) (spectroscopy), Electron Spins Resonance (ESR), Magnetic Resonance Imaging (MRI) in medicine and Giant Magneto- Resistance (GMR) hard drive disk in Computer hard wares.

3. It further establish that the Ising Model is a standard magnetic model used in many areas of research, and is perhaps the most studied model in statistical physics, specifically the 2-D Ising model as it yield to an exact treatment in statistical mechanics which is the only non-trivial example of phase transition without a mathematical rigor.

CHAPTER TWO

LITERATURE REVIEW

2.0 INTRODUCTIONT

The magnetic field of an elementary particle (electron) is an intrinsic field associated with the spin of the particle. The magnetic field can be defined in many equivalent ways based on the effects it has on its environment. Considering a particle having an electric charge *q*, and moving in a B-field with a velocity *v*, experiences a force, *F*, called the Lorentz force which is given by the relation :

$$\vec{F} = q\left[\vec{E} + \left(\vec{v}\, X\vec{B}\right)\right] \qquad (2.0)$$

where, $\vec{E}$ = Electric force.

and $\vec{B}$ = Magnetic force.

Alternatively, it could be defined in terms of the torque it produces on a magnetic dipole.

$$\vec{\tau} = \vec{m}\, X\, \vec{B} \qquad (2.1)$$

where, m = magnetic moment and

$$\vec{B} = \overrightarrow{\mu H} = \frac{\vec{E}}{|v|} \qquad (2.2)$$

where $\vec{H}$ = magnetic strength or interaction.

and $|V|$ = multiplicative constant.

The $\vec{H}$ is defined as a modification of $\vec{B}$ due to magnetic fields produced by material media. Outside of a material (i.e. in vacuum) the $\vec{B}$ and $\vec{H}$ fields are indistinguishable. (They only differ by a multiplicative constant as seen above.). Inside a material, they may differ in relative magnitude and direction with a material dependent multiplicative constant. The Magnetic field at any given point which is a vector is specified by both a direction and a magnitude (or strength).

Magnetization within an atom result from the spin of an electron and its angular momentum wich give rise to magnetic dipole moment and create magnetic field. Quantum mechanically, spin angular momentum is so different from orbital angular momentum. Form the electron's orbital angular momentum one should be able to calculate the B-field (considering the electron as a current). But for spin angular momentum, there is no classical analog to calculate $\vec{B}$ because electron is not actually spinning, rather moving.

2.1 SPONTENEOUS MAGNETIZATION

The appearance of an ordered spin in the absence of an applied magnetic field is the origin of Magnetization in Ferromagnetic materials. Magnetization within an atom result from the spin of an electron and its angular momentum which gives rise to magnetic dipole moment and create magnetic field. Quantum mechanically, spin angular momentum is so different from orbital angular momentum.

Magnetic moment is responsible for magnetization which originated from microscopic electric current resulting from the motion of electrons in atoms, or the spin of the electrons or the nuclei. Net magnetization results from the response of a material to an external magnetic field, together with any unbalanced magnetic dipole moments that may be inherent in the material itself.

Experimentally, magnetic moment is observed by measuring magnetic field generated by the particle. Spin magnetic moment (μ_s) of a particle with charge q, mass m, and spin s is :

$$\overrightarrow{\mu_s} = g\frac{q}{2m}\vec{s} \qquad (2.3)$$

where, g = the g –factor of a dimensionless number.

This number depends on the particle, it characterizes magnetic moment and gyromagnetic ratio (ratio of magnetic dipole moment to angular momentum) of the particle. It is about 2 for electron ($g \cong 2$), for Proton g = 5.586, for neutron g = -3.826 (Paston, 2004, Atherton, 1973). The Proton and neutron are composed of quarks, which have a non-zero charge and a spin of $\hbar/2$ and this must be taken into account when calculating their g-factors. The proton and electron 's spin magnetic moment can be calculated by simply setting q = e. The electron's spin magnetic moment is approximately equal to the Bohr magneton (μ_B)that $g \cong 2$ and not exactly 2. (Atherton,1973: Ewa,1994) and electron spin is $\frac{1}{2}$; thus define the Bohr magneton in the form:

$$\mu_s \approx 2\frac{e}{2m_e}\frac{\hbar}{2} = \mu_B \qquad (2.4)$$

where m_e = mass of electron and ħ = Planck's constant.

2.2 MAGNETIC MATERIALS

Materials can be classified according to their response to externally applied magnetic fields, these magnetic responses differ greatly in strength. Some materials oppose applied magnetic field as such exhibit a very weak magnetic response, such as diamagnetic materials. They induce a weak magnetic field in the opposite direction showing partial anti-alignment.

Some materials produce magnetization in the presence of the magnetic field in the direction of the applied field and proportional to the field, these are paramagnetic materials.

In this work, of interest are the materials that produce a large magnetization in order of magnitude greater than the applied field as a result they are much larger than either diamagnetic or paramagnetic effect (Coey, 2010). These are ferromagnetic materials, they

include a number of crystalline materials such as iron (Fe), Nickel (Ni), Cobalt (Co) and Gadolinion (Gd)) that exhibit ferromagnetism and (non-crystalline) ferromagnetic metallic alloys (such as $FeOFe_2O_3$, $NiO\ Fe_2O_3$, $CuO\ Fe_2O_3$, $MgO\ Fe_2O_3$ etc.)

There are some factors according to Getzlaff, 2010 that determine how materials respond to a magnetic fields. They are : orientation of the spin of an electron in an atom, the orientation of the atoms in a molecule or alloy.

2.3 FERROMAGNETISM IN METALS

Ferromagnetic materials exhibit a long–range ordering phenomenon at the atomic level which causes the unpaired electron spins to line up parallel with each other in a region called a domain(region of magnetic alignment as a result of microscopic ordering of electron spin). The long range order creates the magnetic domain in ferromagnetic materials which arises from a quantum mechanical interaction at the atomic level. This interaction is remarkable in that it locks the magnetic moments of neighboring atoms into a rigid parallel order over a large number of atoms in spite of the thermal agitation which tends to randomize any atomic-level order (Nave, 2010).

Within the domain the magnetic field is intense and this implies that there is already a high degree of magnetization in ferromagnetic materials within individual domains, but in the absence of external magnetic fields those domains are randomly oriented (Nave,2010). Ferromagnetism occurs when externally imposed magnetic field cause the magnetic domains to line up with each other and the material is said to be magnetized.

Ferromagnetic materials, such as iron, contain unpaired electrons, each with a small magnetic field of its own, that align readily with each other in response to an external magnetic field. This alignment tends to persists even after the magnetic field is removed, a phenomenon

called hysteresis. The fraction of the saturated magnetization which is retained when the driving field is removed is called the remanence of the material, and is an important factor in permanent magnets (Nave,2010). Ferromagnetism is also important in the design of electromagnets, transformers, and many other electrical and mechanical devices.

The long range order phenomenon in Ferromagnetic materials can abruptly disappear due to thermal agitation at a certain temperature known to be Curie temperature of the material. The Curie temperature gives an idea of the amount of energy it takes to break up the long-range ordering in a certain material. The Curie temperature of iron is about 1043 K. At 1043 K the thermal energy is about 0.135 eV compared to about 0.04 eV at room temperature.(Nave.2010). A little above the Curie temperature a ferromagnetic material tend to lose it ferromagnetism and become paramagnetic.

It is of importance to note that ferromagnetism is a property that is due to the direct influence of two effects from quantum mechanics and that is spin and Pauli Exclusion Principle. The spin of an electron in the atoms is the main source of ferromagnetism (Bozorth, 1993).

2.4 ELECTRON SPIN DISTRIBUTION

Since the discovery of electron spin in 1924 by Wolfgang Pauli it was clear that magnetism exist as a result of large number of electrons spinning in the same direction, this is so because the electrons on one side of a magnet do not directly interact with the electrons on the other side, they only influence their neighbors. The Spin was discovered in the context of emission spectrum of alkali metals which informed him (Wolfang Pauli) to introduce what he called a "two-valued quantum degree of freedom" associated with the electron in the outermost shell and this two-value quantum degree of freedom is the spin. The spin is symbolized by (S) and

is often followed by a "+" positive sign or "-" negative sign. This refers to the parity with "+" for even parity and "-" for odd parity (Wolfgang, 1940).

The spin has a quantum number of $s = n/2$, where n is any non negative integer with allowed values of s as 0, 1/2, 1, 3/2, 2, etc. The value of s for an elementary particle depends on the type of particle, and cannot be altered in any known way (Wolfgang, 1940). The spin angular momentum S of any physical system is quantized with value of S as :

$$s = \hbar\sqrt{s(s+1)} \qquad (2.5)$$

where; $\hbar$ = the reduced Planck's constant.

All known matter is ultimately composed of elementary particles called fermions, and fermions have s = ½. Example of fermions is the electron and electron spin s = 1/2 is an intrinsic property of the electrons.

Atomic nuclei usually has total angular momentum which is made up of sum of the spins and orbital angular momenta of the constituent particle. Such a composite spin is subject to the same quantization condition as any other angular momenta. Spins have some peculiar properties that distinguish them from orbital angular momenta. These properties are :

- Spin quantum numbers may take on half-integer values as seen above.
- Although the direction of its spin can be changed, an elementary particle cannot be made to spin faster or slower. By way of classical mechanics the angular momentum of a particle possesses not only a magnitude , but also a direction (either up (↑) or down(↓) on the axis of rotation of the particle).

Quantum mechanics has also proved that spin also contains information about direction, but in a more subtle form. Therefore the component of angular momentum measured along any direction (say along the *z*-axis) can only take on the values of $\hbar s_{z,}$ where

$$S_z = -s, -s+1, \ldots\ldots, s-1, s \qquad (2.6)$$

s is the principal spin quantum number.

From eqn. 2.6 there are $2s+1$ possible values of s_z. The number "$2s+1$" is the multiplicity of the spin system. In these research work there are two possible values for a spin (s) – 1/2 particle (which is electron) i.e $s_z = +1/2$ and $s_z = -1/2$. These correspond to quantum state in which the spin is pointing in the +z or −z directions respectively, (spin ↑ and spin ↓). For a given quantum state, there is a need to describe a spin vector {S} whose components are the expectation values of the spin components along each axis in space.

$$(s) = [(s_x), (s_y), (s_z)] \qquad (2.7)$$

This vector describes the direction in which the spin is pointing, corresponding to the classical concept of the axis of rotation. The spin vector cannot be measured directly, i.e. s_x, s_y and s_z cannot possess simultaneous definite values, because of a quantum uncertainty relation between them. However, for statistically large collections of particles that have been placed in the same pure quantum state, such as through the use of a Stern - Gerlach apparatus the spin vector does have a well-defined experimental value. Which specifies the direction in ordinary space in which a subsequent detector must be oriented in order to achieve the maximum possible probability (100%) of detecting every particle in the collection. For spin-1/2 particles,

this maximum probability drops off smoothly as the angle between the spin vector and the detector increases, until at an angle of 180 degrees, that is, for detectors oriented in the opposite direction to the spin vector—the expectation of detecting particles from the collection reaches a minimum of 0% (Weinert, 1995). Thirdly, The spin of a charged particle is associated with a magnetic dipole moment and a g-factor as discussed under magnetization.

One other interesting property of the spin it is associated with is eigenvectors just as with orbital angular momentum and the spin obeys commutative relations analogous to those of the orbital angular momentum in the following order :

$$[s_i , \ s_j] = i\hbar\epsilon_{ijk}\, s_k \qquad (2.8)$$

where: ϵ_{ijk} is the permutation symbol. And *ijk* are the index of permutation. ϵ_{ijk} can either be = 1 or = -1. If it is equall to 1 then the index (*i*, *j*, *k*) is an even permutation of (1,2,3), and if the index is equall to −1 then the index (*i*, *j*, *k*) is an odd permutation, and ϵ_{ijk} could be zero (0) if any index is repeated (Fowler, 2007).

These eigen vectors are s^2 and s_z (expressed as kets in the total (S)basis) as expressed below :

$$s^2|s,m\rangle = \hbar^2\, s(s+1)|s,m\rangle \qquad (2.9)$$

$$s_z|s,m\rangle = \hbar m|s,m\rangle \qquad (2.10)$$

The spin raising and lowering operators acting on these eigenvectors give:

$$s_\pm|s,m\rangle = \hbar\sqrt{s(s+1) - m(m\pm 1)}\,|s,m\pm 1\rangle \qquad (2.11)$$

where $s_{\pm} = s_x \pm is_y$ (2.12)

Unlike orbital angular momentum the eigenvectors are not spherical harmonics as such they are not functions of θ and ϕ.

There is an interaction (electrodynamics) between spin of an electron and its motion (the spin orbit coupling) which leads to a shift in an electron atomic energy levels as a results of temperature change which is synonymous to phase transition. In a phase transition of a given medium certain properties of the medium changes, often discontinuously, as a result of some external condition, such as temperature and pressure. In the case of ferromagnetic materials under a temperature above the curie temperature, symmetry is broken and the state changes to a paramagnetic one, (ferromagnetic-paramagnetic transition, loss of magnetic order) this change in state require the introduction of one or more extra variables to describe the state of the system, such variable are examples of order parameters (a measure of the degree of order in the system) : the extreme values are 0 for total disorder and 1 for complete order (Kleinert, 1989).

Ferromagnetic materials have order parameters for more than one degree of freedom. In this case the order parameter may take the form of a complex number, a vector, or even a tensor, the magnitude of which goes to zero at the phase transition, these necessitate formalizing relationships between these variables in the form of mathematical equations with the aid of a statistical model.

2.5 THE ISING MODEL

An Ising Model is a model of a magnet, where some geometry is chosen to represent the individual magnetic dipole moments of the constituents of the material in question. The combined individual moments produce an overall magnetization in the entire material.

It mathematically model ferromagnetism in statistical mechanics and it is the simplest theoretical description of ferromagnetism. This model was invented by Wilhelm Lenz in 1920 and named it after Ernst Ising, a student of his (Lenz) who chose the model as the subject of his doctoral dissertation in 1925. It is a simplified model of phase change in real substance which has been use to model diverse phenomena in which bits of information interacting in parts produce collective effects.

This model consists of spins (s_{ij}) as discrete variables which exist in one of two state (+1 or -1). The spins are arranged in a lattice (Λ) (with $\langle ij \rangle$ per each lattice site) or graph and each interact with its nearest neighbors. The basis for this arrangement is to find phase change in the Ising model. Given a transitional invariant interaction of I_{ij} and a point dependant field H, the Ising model has a configuration energy of :

$$E_I(s_i) = \sum_{\langle ij \rangle} -J_{ij}\, s_i s_j - \mu H \sum_{i=1}^{N} s_i \qquad (2.13)$$

where, $\langle ij \rangle$ denotes a nearest-neighbor pair of spins and the subscript *I* stands for Ising model.

i = 1, ….., N) which is a number that is either +1 or -1.

J_{ij} = is the interaction energy of the system.

μ = is the magnetic moment.

H = Represent the external magnetic Field. the J_{ij} and H are given constant.

The sum over $\langle ij \rangle$ contains a term $\boldsymbol{\gamma}\frac{N}{2}$, where $\boldsymbol{\gamma}$ is the number of nearest neighbors of any given site which gives the lattice its geometry alongside the interaction energy. This is possible because $\boldsymbol{\gamma}$ can be expressed in different geometrical form as follows:

$$\gamma = \begin{cases} 4\ (two \quad dimensional\ square\ lattice) \\ 6(three - dimensional\ simple\ cubic\ lattice) \\ 8(three - dimensional\ body - centered\ cubic\ lattice) \end{cases} \qquad (2.14)$$

The interaction of the spin with an external magnetic field tend to align all spins in the same direction. Magnetic Interaction seek to align spin relative to one another and get randomized when thermal energy is greater than the strength of interaction. For each pair of interaction, if $J_{ij} > 0$ the interaction is refered to as Ferromagnetic, if $J_{ij} < 0$ the interaction is anti-ferromagnetic and for $J_{ij} = 0$ the spins are non-interacting.

2.6 THE 2-DIMENSIONAL ISING MODEL

In solving the Ising model, Wilhelm Lenz in 1920 gave it as a problem to his student Ernst Ising after whom it was named who worked on the 1-Dimensional model in 1925. On the basis of his result, he concluded that his model does not exhibit phase behavior in any dimension.

The Model was later worked on by Lar Onsager in 1944 where he formulated the two – dimensional Ising model in terms of matrices as a preliminary step towards an exact solution of the model, using a method of transfer- matrix in 2-Dimension analytically in zero magnetic field and he discovered that the Ising model undergoes a phase transition between an ordered and a disordered state (Osanger, 1944).

In the Osanger solution a square lattice of $N = n^2$ spins consisting of n – rows and n –column with an enlargement by one row and one column with the configuration of the (n +1)th row

and column (identical with that of the first row and column respectively) as a boundary condition was considered as shown below:

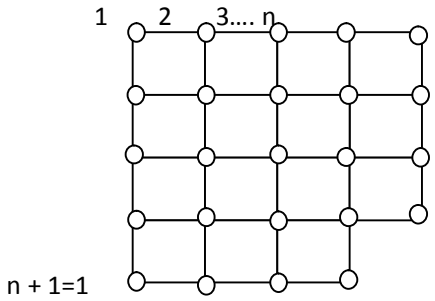


Figure 2.0 lattice presentation of Two- dimensional Ising model

This boundary condition endows the lattice with the topology of a torus as shown in figure 2.1.

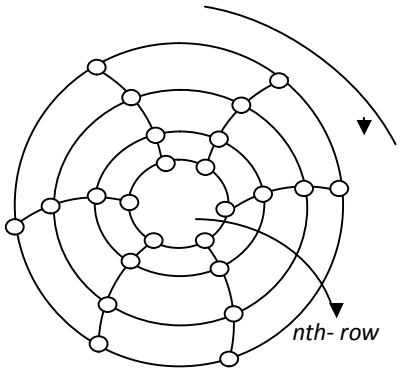


Figure 2.1 Topology presentation of the two-dimensional Ising model

with $\mu_x \quad (x = 1, \ldots \ldots, n)$ as the collection of all the spin coordinates of the α^{th} row.

$$\mu_x \equiv \{s_1, s_2, \ldots\ldots, s_n\}\alpha\text{th row} \qquad (2.15)$$

The configuration of the entire lattice is specified by $\{\mu_1, \ldots\ldots, \mu_n\} \ldots\ldots\ldots\ldots$

The α^{th} row is assumed to interact only with $(\alpha - 1)^{th}$ row and $(\alpha + 1)^{th}$ row. Therefore the energy of the 2-D Ising model is made up of the interacting energy between the α^{th} and the $(\alpha + 1)^{th}$ row which is

$$E(\mu, \mu') = -J \sum_{\alpha-1}^{n} s_\alpha s'_\alpha \qquad (2.16)$$

$$\mu = \{s_1, \ldots\ldots, s_n\} \qquad (2.17)$$

$$\mu' \equiv \{s_1', \ldots, s_n'\} \qquad (2.18)$$

$$s_{n+1} \equiv s_1 \qquad (2.19)$$

where μ_α and $\mu_{\alpha+1}$ are collection of spin coordinates in two neighboring rows, and

J = interaction energy. Equation 2.11 hold for the boundary condition in each row.

Interacting energy of the spins within the α^{th} row plus their interaction energy with an external magnetic field is given.

$$E(\mu) = -J \sum_{\alpha=1}^{n} s_\alpha s_{\alpha+1} - B \sum_{\alpha=1}^{n} s_\alpha \qquad (2.20)$$

where , B = external magnetic field.

The total energy of the lattice for the configuration $\{\mu_1, .., \mu_n\}$ is then

$$E_I\{\mu_1, .., \mu_n\} = \sum_{\alpha+1}^{n} [E(\mu_\alpha, \mu_{\alpha+1}) + E(\mu_\alpha)] \qquad (2.21)$$

with its partition function to be

$$Q_I(B, T) = \sum_{\mu_1} \ldots\ldots \sum_{\mu_n} e^{-\beta E_I\{\mu_1, \ldots\ldots, \mu_n\}} \qquad (2.22)$$

where; β = reduce Boltzmann constant at a reduced temperature T.

This partition function now becomes the element of a defined $2^n \times 2^n$ matrix that will be expanded using Kaufman's generalization of Onsager's solution in which exact distribution function for the energy can then be determined using mathematical rigor which involves a polynomial. Expansion using binomial series in order to explicitly remove all squares that

might hide the polynomial nature of the final result . A final verification of the correctness of the calculation will be needed so as to ensure that the reduced free energy per spin gives the same power series as the thermodynamic limit series.

The correctness or accuracy of the above calculation cannot be ascertained due to the fact that the Ising model is a crude attempt to simulate the structure of a physical ferromagnetic substance. Therefore there is the need to use the Monte Carlo simulation because the histograms of energies that will be generated from Monte Carlo simulations will be compared with this exact distribution.

2.7 THE MONTE CARLO METHODS

Numerical methods that can be used to describe statistical simulation which are concerned with the use of sequencing of random numbers are known as the Monte Carlo methods. Historically the name "Monte Carlo" was coined by Metropolis (inspired by Ulan's interest in poker) during the Manhattan Project of World War II (cerena@xsep1.phy.gov) in reference to the famous casino in Monaco. Monte Carlo is now of tremendous use in many diverse fields, from the simulation of complex physical phenomena such as radiations transport in the earth's atmosphere and the simulation of the esoteric sub-nuclear processes in high energy physics experiments to production systems and also space exploration.

Statistical simulation method differ from conventional numerical methods which typically are applied to ordinary or partial differential equation that describe some underlying physical or mathematical system. In many application of Monte Carlo, the physical process is simulated directly without a differential equation that describes the behavior of the system. The only

necessary requirement is that the system be described by a probability density function (PDF). Once this is applicable the statistical simulation can proceed by random sampling from the PDF and many trials are performed. The desired result is taken as an average over the number of observations. In many practical application, one can predict the statistical error in this average result, and hence an estimate of the number of Monte Carlo trials that are needed to achieve a given error.

If a system can be described by probability density function then the Monte Carlo simulation can proceed by sampling from these PDF's which necessitate a fast and effective way to generate random numbers uniformly distributed on the interval $[0,1]$. The outcome of these random sampling must then be accumulated in an appropriate manner to produce the desired result, but the essential characteristic of Monte Carlo is the use of random number (and perhaps other algebra to manipulate the outcomes) to arrive at a solution of the physical problem. In contrast, a conventional numerical solution approach would start with the mathematical model of the physical system, discrediting the differential equation and then solving a set of algebraic equations for the unknown state of the system.

2.8 THE STRATEGY OF MONTE CARLO METHODS

Essentially at each step in the evolution of the calculations, the probability of a potential transition is calculated. A random number (between 0 and 1) is selected (using standard programs like the translator) that can be found on most computers. If the calculated probability exceeds the selected random number, the potential transition is performed, otherwise if the calculated probability is less than the random number the potential transition is ignored and a new one is tried instead.

The basic Monte Carlo procedure of simulating phenomena through a number of random simple steps is often the only realistic way of performing calculations in large complicated

systems , system with large number of degrees of freedom. Among these are the many atoms in chunk of condense matter as in many electrons in an atom. The description of such systems is often involve atoms at a temperature 1/β interacting through a pair-wise potential v which is proportional to the three dimensional integral given as

$$Z = \int d^3 r_1 \dots \dots d^2 r e^{-\left[\beta \Sigma_{i<j} v\left(\overrightarrow{r_{ij}}\right)\right]} \qquad (2.23)$$

The quantum Monte Carlo methods employed in this work are ways of specifying the energy for each possible state of the system, while the Boltzmann function gives the probabilities of the system to be in each states(at some specified temperature). Therefore microscopic quantities of interest can be calculated by doing simple probabilities sums.

To clarify the meaning of "probability sums" consider the problem of calculating the (average) magnetization of the system. For any fixed state S, the magnetization is proportional to the "excess" number of spins pointing up:

$$M(S) = N_{\uparrow}(S) - N_{\downarrow}(S) \qquad (2.24)$$

To evaluate the average magnetization of the whole system, we simply sum up these values over all the possible states, weighting each state by the (Boltzmann) Probability that the state actually occurs.

$$Expectetd\ magnetization = \sum_{s} M(s)P(s) \qquad (2.25)$$

This looks simple enough, but the calculation is completely hopeless due to the number of terms in the sum. The relationship between the number of sites in the "Ising universe" and the number of different states of the system is;

[N Lattice Sites] => [2^N Different States] (2.26)

(Two orientation at the first site time, two orientations at the second site times)

The 2^N behavior for the number of states could be a complete computational problem for a small 16 x 16 lattice (256 total sites), there are about 10^{77} different states in the probability sum. To expantiate this further, a really fast computer might be able to evaluate about 10^{10} individual terms per second, and the entire calculation would be completed in about 10^{67} seconds. this could be more appreciated if the universe is known to be about 10^{20} seconds or 317,097,919,838 years old. For now there are two qualitative reasons why the Monte Carlo simulation is a reasonable procedure for estimating average quantities for interacting system:

1. The procedure does not waste time /effort generating or examining improbable configurations.
2. Rather than exploring all configurations – including enormous numbers of configurations which are extremely similar in terms of microscopic quantities – the algorithm meanders along a modest number of representative paths.

The procedure randomly samples states according to the real underplaying probability distribution. This in turn makes it possible to estimate system average with reasonable sized simulation samples.

2.9 METROPOLIS - HASTINGS ALGORITHM

The Metropolis – Hastings Algorithm is a mainstay of scientific computing. Indeed it appears first on a list of "top ten Algorithm" (Persi, 2004). It has been proven to be the famous way of generating random variables with a given probability distribution of arbitrary form (Koonin, 1989). This algorithm provides a method for sampling from probability distributions on high – dimensional spaces that round up to a normalizing constant. This algorithm has been applied widely in statistical mechanics problems where the weight function of the canonical ensemble is a complicated function of the coordinates of a system.

The Algorithm works based on a sample realization of say : generating a set of points in a space (possibly multi –dimensional) of variable X distributed with probability density W(X). If X_0 , X_1 ……, are point visited successfully by a random walk moving through X – space, the work becomes longer and longer, the point it connect approximate more closely to the desired distribution. The rules by which the random walk proceeds through configuration space are as follows:

Suppose the walker is at a point X_n in the sequence. To generate X_{n+1} it makes a trial step to a new point X_t. This new point can be chosen in any convenient manner, for example uniformly at random within a multi – dimensional cube of small side δ about X_n this trial step is then accepted or rejected according to the ratio

$$r = \frac{w(X_t)}{w(X_n)} \qquad (2.27)$$

If r > 1 then the step i is accepted (i.e $X_{n+1} = X_t$) but if r < 1, then the step is accepted with probability r. r can be conveniently compared with a random number η uniformly distributed in the interval $[0,1]$ and accepting the step if η < r. If the trial step is not accepted then X_{n+1}= X_n which means X_{n+1} is generated and we may proceed to generate X_{n+2} by the same process, making a trial step from X_{n+1}. Any arbitrary point, X_0 can be used as the starting point for the random walk. These points are not independent of one another and this is so due to the manner in which they are generated, that is, X_{n+1} is likely to be in the neighborhood of X_n.

Points in space must be distributed properly. This is necessary as the work becomes very long and the points are not statistically independent so that the integral calculation can be performed to get a realistic result. For instance calculate

$$I = \frac{\int dX\, w(X) f(X)}{\int dX\, w(X)} \qquad (2.37)$$

and

$$C(k) = \frac{\langle f_i\, f_{i+k}\rangle - \langle f_i\rangle^2}{\langle f_i\rangle^2 - \langle f_i\rangle^2} \qquad (2.38)$$

where $\langle \ldots\ldots \rangle$ indicates average over the random walk.

and

$$\langle f_i\, f_{i+k}\rangle = \frac{1}{N-k} \sum_{i=1}^{N-k} f(X_i)\, f(X_{i+k}) \qquad (2.39)$$

By averaging the values of *f* over the point of the random walk, the usual estimates of varience is invalid because the *f* (X_i) are not statistically independent. This can be quantified by calculating the auto – correlation function in equation 2.38.

It is a known fact that $C(0) = 1$, but the non – vanishing of *C* for *k* at $k \neq 0$ means *f's* are not independent. In practice, appropriate starting point is a probably where w(X) is large but some number of thermalization steps can be taken before actual sampling begins to remove any dependence on the starting point.

2.10 MONTE CARLO SIMULATION

Instead of sampling (measuring parameters like expectation values) for a lot of states and then weighting them by their Boltzmann factors, it makes more sense to choose states based on their Boltzmann factors and to then weight them equally using the Metropolis algorithm, which involves a pseudorandom number generator which is an important sampling technique. This is exactly what the Monte Carlo simulation does. And One random pass through the algorithm is described as:

1. A trial configuration is made by randomly choosing one spin.

2. The energy difference of the trial state relative to the present state, δE, is calculated.

3. If $\delta E \leq 0$, the trial state is energetically favorable and thus accepted. Otherwise, a random number $0 \leq \eta \leq 1$ is generated, and the new state is only accepted if $e^{-\beta \delta E} > \eta$.

If the expectation value for an observable state say A, is

$$\langle A \rangle = \frac{\sum_r A_r \, e^{-\beta E_r}}{\sum_r e^{-\beta E_r}} \qquad (2.40)$$

where A_r is the expectation value of (A) for the state (r) according to (Lisa, 2002) and E_r is the energy of the state.

Given a system that has a discrete number of states, we could, using a computer calculate A for each state and weight these values by their Boltzmann factors to find the average A. This might be feasible for a system with a small number of states, but if we have say a 20 x 20 spin lattice interacting via the Ising model, there will be 2^{400} states, so we cannot possibly examine all of them. But what if we decide to just sample some of the states, how would we decide which ones to sample?

One conventional way of using random numbers was to randomly pick a lot of states, measure <A> for each of them and weight these values of <A> by their Boltzman factors. These might get close to the right answer if a lot of states were sampled , but we would spend a lot of time calculating < A> for states that contribute very little to the final result and an Ising lattice at very high temperature is unlikely to be in the state where all spins point in one direction. This is where the Monte Carlo simulation comes in. The simulation provides a clear spin array which provides accurate observable information on how the temperature relates with spin alignment. For high temperatures, the spins remain randomly aligned after long periods of

equilibration, whereas for low temperatures, the spins end up pointing in mostly the same direction.

This simulation allows energy and the magnetization to be measured at each step of the sub routine by allowing the system to equilibrate for a long time and then measure the magnetization by taking the sum of all the spins in the lattice, calculate the energy by determining the energy for each spin and dividing by two for double counting. Similarly the simulation calculates the specific heat capacity in terms of the variance of the energy and magnetic susceptibility in terms of the variance in the magnetization. All these has eliminates the cumbersomeness of partition function derivative.

2.11 RELATED PREVIOUS WORKS

The Ising model was treated similar to the case of isotropic interactions by Ceperly *et'al* in 1979 where all the interaction energy (J_{ij}) were made to be equal to a single number (J) which reduces the configuration energy from equation 2.13 to

$$E_I(s_i) = -J\sum_{(ij)} s_i s_j - \mu H \sum_{i=1}^{N} s_i \qquad (2.41)$$

Such that it can arrive at its partition function as given in equation 2.22

where H = is the Hamiltonian for single state , β = 1/kT and μ in equation 2.41 is collection of spin coordinates, which will in turn be used to get the thermodynamic functions of ferromagnetism (which are internal energy, heat capacity and magnetization.) using the Helmholtz free energy of (Ceperley, 1979).

$$A_i(B,T) = -kTlogQ_i(B,T) \qquad (2.42)$$

2.11.1 EXACT DISTRIBUTION OF ENERGIES IN THE TWO-DIMENSIONAL ISING MODEL

The low-temperature series expansion for the partition function of the two-dimensional Ising model on a square lattice was determined exactly for finite lattices using Kaufman's generalization of Onsager's solution (Beale.1995).

The exact distribution function for the energy was determined from the coefficients of the partition function. This was done by considering an isotropic two-dimensional Ising model with nearest-neighbor interactions on a lattice with *m* rows and *n* columns with periodic boundary conditions in zero external field that is defined by the Hamiltonian

$$H = -J \sum_{ij} s_i s_j \qquad (2.43)$$

where $s_i = \pm 1$ and J is the coupling energy and the sum is over pairs of nearest-neighbor sites on the lattice. With the partition function at any temperature *T* at a low-temperature series expansion of :

$$Z_{n,m}(K) = e^{2nmk} \sum_{k=0}^{nm} g k X^{2k} \qquad (2.44)$$

where $K = {}^{J}/_{k_B T}$ is the coupling, k_B is the Boltzmann's constant and $x = e^{-2k}$ is the low-temperature expansion variable, and the coefficient *gk* is the number of configurations with energy 4*kJ* above the two ground states.

2.11.2 ELECTRON SPIN RESONANCE TECHNIQUE

Electron Spin Resonance (ESR) is one of the analytical methods used in the characterization of paramagnetic species as applicable check in it crystal field characterization which has been

outlined through the fundamental concept of the precessional motion of electrons and their magnetic moment at resonance as carried out by Ewa, 1994.

The interaction of an ion in a crystal field in paramagnetic studies is a fruitful application of ESR in field characterization of transition element, since these groups of elements preserve their unfilled electron shells during crystal formation. Excellent work on relaxation phenomenon associated with paramagnetic species of the 3dn transition group with a focus on localized O_2species within a T_iO_2 crystal field when subjected to an irradiation with an appropriate resonance frequency could be referred to (Ewa, 1994).

2.11.3 DACAPO CALCULATION OF MAGNETIC PROPERTIES OF FERROMAGNETIC MATERIALS

It can be difficult finding out the lowest energy of a magnetic state. In some cases one may wonder which is more stable, a ferromagnetic state or non-magnetic solution. A major discovery reveals there are many different ways to arrange spins on the various atoms in a geometry. One approach is to reduce the complexity by fixing the total magnetic moment of the unit cell and let the spins go to any direction; the idea is to calculate the total energy versus unit cell magnetic moment to identify minima (Moroni, 1997).

This was done by a computer program written in Dacapo and run on Python via Jacapo interface to calculate the bulk magnetic moment of Fe.

2.11.4 THE STUDY OF 2-D EDWARDS-ANDERSON SPIN GLASS USING MONTE CARLO METHODS.

In this particular study, the Monte Carlo methods was applied to study two dimensional Edwards- Anderson spin glass using an optimized algorithm that considers localized event of the Markov chains particular to singly affected sites in the single spin- flip dynamics (Igwe *et'al,* 2011). Consequently they obtained result for large system size up to 515 x 512 (i.e N =

n^2 where n = 512) by performing the simulation over a range of temperature $0 < k_B \leq 8$; for 50 different realizations which is adequate to greatly reduce statistical fluctuation.

2.12 LIMITATIONS OF PREVIOUS WORK

The low-temperature series expansion for the partition function of two-dimensional Ising model cannot be concluded as the solution that gives exact energy distribution per spin, due to the fact that there was a reduction in free energy of the system due to uncertainty.

While the ESR technique is regarded as a rapid non-destructive and extremely sensitive method for crystal field studies, it should be noted that the investigation of the adsorbed species within a crystal field could yield complicated line intensities and structure. ESR technique is limited in the way that it is only applicable to paramagnetic substances, a such it could not be said to be a universal application of magnetic field effect.

The Jacapo program used in calculating the magnetic properties of ferromagnetic system is unable to calculate the energy for a magnetic moment of zero and was limited to just the magnetic moment from one upward. Each time the program is run for zero, a zinsc2 error appears which is known as the Bayesion error analysis, due to the fact that it has an estimated value for energy and magnetic moment.

CHAPTER THREE

METHODOLOGY

3.0 INTRODUCTION

The Monte Carlo simulation program is the main method used in this research work. The simulator is a computer program written and complied in FORTRAN 90, an acronym for Formula Translation (Koonin, 1989). There are four categories of files that makes up the whole simulation package: the source code, common utility, data codes and the include codes.

The simulation work in accordance with the Metropolis Algorithm. The algorithm uses the Hamiltonian,

$$H = -J\sum_{ij} S_i S_j - h\sum_{i} S_i \qquad (3.0)$$

where j = interacting strength between lattice sites (coupling energy)

$\langle ij \rangle$ = sum over nearest neighbor

s_i = spin at single site

h = external energy

- To determine the configuration energy.
- To flip the spin at the selected site and recompute the configuration energy by taking the difference between the initial energy at start scan and the final energy at finish scan.
- If the difference is less than zero, then it will allow the spin to flip which will give rise to a randomly generated number that is less than the Boltzmann factor $e^{-\beta \triangle E}$ where $\beta = {}^{1}/_{kT}$

3.1 THE SOURCE CODE

The source code is organized in subroutines or modules, each performing limited and well defined tasks. The ARCHON subroutines that perform the calculation are at the beginning of the code with a header that describes the purpose of the subroutines and the variables it uses. That is : input variable and output variables, declaration where variable are defined, (which are passed to the subroutines in the call statement), LOCAL variables (which are used only within that subroutine) and GLOBAL variables (which are pass in common blocks). FUNCTION (which define FORTRAN functions).

3.2 THE INPUT VARIABLES

The input parameters are of two categories; they are the physical parameter and the numerical parameter which make up the bulk input parameters. They are stored in 'ising.in' which is an in-built file which allow the size, length, and initial configuration of the simulation to be changed at the point of execution.

The magnetic field, integration strength, number of thermalization sweeps, sweep frequency and group size are inputted manually taken from a range of figures provided by Ising. The 'ising.in' contains spin, number of passes for each temperature, number of equilibrium steps, temperature of scan start, temperature of scan stop, scanning interval (interval between scan points), configuration type, check board and interface of a magnetic material. The file contains the following parameters.

Table 3.1 : Inputs parameter from ising.in file

INPUTS NAME	INPUTS VALUE
Spin.	20 rows , 20 columns
Number of passes for each temperature.	200000
Number of equilibrium steps.	100000
Temperature of Scan Start.	2.92K
Temperature of scan finish.	0.92K
Scanning Interval.	0.1
Configuration type.	1
Checker board.	2
Interface.	3
Unequal Interface.	1

Table 3.2 : Manual Inputs parameters

Magnetic field (kT).	0.001 x10^{-1} kT	Ranges 0.1 -0.3
Interaction strength (kT).	0.3 x 10^{-3}	1000 – 3000
Number of lattice point.	X = 20 Y =20	Maximum of 20
Integer Random number seedfor initial Fluctuation.	1000	$0 \leq N < 1$
Number of Thermalization sweeps.	20	Maximum of 20
Sampling frequency to avoid correlation.	5	Maximum of 5
Number of Sample in a group.	10	Maximum of 10
Group size.	10	Maximum of 10

The complied code has the programmer work bench (PWB) which is divided into seven which can be 'called' independently. It has the menus for changing physical parameters, changing numerical parameters, changing output parameters, displaying physical and numerical parameters, displaying output parameters, menu to run the code and to stop the code.

The METROP subroutine: these calculate one sweep of the lattice using the Metropolis algorithm to generate a new configuration for spin and acceptance ratio. Then the SUM subroutine which calculates spins, magnetization and energy of a particular sweep and add these values to the group average. Similarly, we have the AVERAG subroutine which finds the group averages from group sums and add these to total averages and calculates uncertainties.

The INIT subroutine initializes constants, displays header screen and initializes menu arrays for input parameters. The PARAM subroutine gets parameters from screen, ends parameters on screen, closes old files, maps menu variables to program variables, open new files, calculates all derivative parameters and perform checks on parameters. The PRMOUT, DISPLAY, SWPOUT, TITLES subroutine keep calls to subroutines as uncluttered but as informative as possible. Variables that are constant for one run are passed in common blocks.

3.3 THE COMMON UTILITY, DATA AND INCLUDE CODES

The code contains three main files: UTIL. FOR, SETUP.FOR and GRAPHIT.BLK. these files are called by and therefore must link with the source code. UTIL.FOR contains the routines for menu, I/O, file opening /closing e.t.c. SETUP.FOR contains all variables and routines that are hardware and compiler dependent e.g. screen length and terminal unit number. (This file can be edited to get the most efficient and attractive output). GRAPHIT.BLK contains empty subroutines for non-existence package. This file is included so that there are no unsatisfied

calls at link time. There are three data files all have . DAT extension and contain default data that can be read into the source code at run time where an input is not supplied. The last category of the file in the package is the include files which contains common blocks and variables type declarations that must be included in the FORTRAN source code to compile them.

3.4 CODE EXECUTION

The 1st stage of the simulation is accepting the input files and changing the initial configure ation for size, length and spin. Then the setting of the spin matrix dimensions by the use of a periodic boundary conditions. The conditions are: The first two rows and columns must be the same as the last two and the n-rows and n-column have to be even. This is to ensure that the first two rows/cols start out the same as the last two.

The 2nd stage is the execution of the Main loop containing Monte Carlo algorithm. It begins by calling the accepted input parameters from the " ising.in" file and input device. loop spin array are computed (written to an output file each time it is computed) and the outcome compared (tested) with the equilibrium steps for each temperature. If the spin array is greater than the equilibrium steps, the magnetization and energy of that spin is calculated. Otherwise the loop will increase its count by 1 and repeat the process over again. The energy is then divided by the number of spin to get the average energy per spin and the result is divided by two to account for double counting.

The 3rd stage is a loop for random number generating function where a trial configuration is made by randomly choosing one spin change in order to get change in energy due to the trial move. The energy difference of the trial state relative to the present state, δE, is calculated. If

$\delta E \leq 0$, the trial state is energetically favorable and thus accepted. Otherwise, a random number $0 \leq \eta \leq 1$ is generated, and the new state is only accepted if $e^{-\beta \delta E} > \eta$. β is the inverse energy and the final spin - array (containing a snap shots of spin lattice) with it associated temperature, Magnetization (susceptibility) and Energy will now be written to an output file as the final output.

The 4th stage is the simulation proper which allow the magnet to start in a randomized state, and subsequent time translations are governed by a daemon that visits each site on the lattice exactly once. The daemon starts at a random site, and jumps by number of lattice sites (wrapping around the lattice when necessary).

The local energy of the current site is determined through the four nearest neighbors, which are ferromagnetically coupled. Each neighbor interaction contributes a factor of -1 for aligned spins, and +1 for anti-aligned spins. The daemon will flip the spin if that will lower the energy. If not, the daemon will only flip the spin with a probability of the Boltzmann factor $e^{-\beta \Delta E}$ where delta E is the difference between the flipped and the unflipped energies.

The average spin at each lattice point generate individual magnetic dipole moments (generated by "nearest-neighbor") meaning only those sites on the lattice that are exactly one lattice-spacing from a chosen site is considered. It can also be deduced that much localized ordering (sites with nearest-neighbors) can lead to much larger scale ordering on the entire lattice. This models the phenomena that the combination of individual dipole moments generates a net magnetization throughout the bulk of the material. In order to enhance the analysis and to comprehend the effect of lattice size on spin distribution, the simulation was

carried out for 2 X 2 lattice and repeated for 3 X 3 lattice, 4 X 4 lattice, 5 X 5 lattice and 20 X 20 lattice points.

The thermalization sweeps are carried out in group of 10s such that each group has ten (10) thermalization sweeps with its acceptance ratio; the average is taken as an average value for the thermalization sweep for that particular group. For each lattice point there are about ten groups labeled as G1, G2, G3, , ……G10.

This simulation gives energy and the magnetization to be measured at each step of the sub routine by allowing the system to equilibrate for a long time and then the magnetization is measured by taking the sum of all the spins in the lattice, the energy is calculated by determining the energy for each. The end result of the code are for a range of temperatures that is determined by the number of thermalization sweep and the spin – array containing snapshots of the spin lattice at the end of each temperature run.

CHAPTER FOUR

RESULT ANALYSIS AND DISCUSSIONS

4.0 INTRODUCTION

The output of the simulation code are in two forms, the first categories is the spin snapshot and the second one are the numerical values of the various thermodynamic variables obtained per spin.

4.1 RESULT

We have obtained qualitative information from the simulation by watching array of spins, the information were generated as average values for Energy, Magnetization, Susceptibility and Specific Heat Capacity per spin for a range of temperatures that is determined by the number of thermalization sweep for each lattice points and the spin – array display containing snapshots of the spin lattice represented in Matrices.

4.2 SIMULATION OF SPIN ALIGNMENT FOR 2 X 2 CRYSTAL LATTICE.

Below is the spin –array display that was obtained on running the code foe 2 x2 lattice structure under the condition of magnetic field of 0.0001 kT , interacting strength of 0.300 kT ten thermalization sweeps and ten groups respectively. The spin snapshot was presented in matrices in order to obtained accurate and precise result.

Group 1

 sweep1 E = -0.600, M= -1.000  sweep2 E= -0.600,M= 1.000

 sweep3 E = -0.600, M =1.000  sweep4 E= --0.600, M= -1.000

 sweep5 E= -0.600, M = -1.000  sweep6 E = -0.600, M = -1.000

 sweep7 E= 0.000, M = 0.5000  sweep8 E = - 0.600, M = -1.000

 sweep9 E= - 0.600, M = -1.000  weep10 E = -0.600, M = 1.000

Group 2

 sweep1 E = -0.600, M= 1.000  sweep2 E= -0.600,M= -1.000

 sweep3 E = 0.000, M = - 0.5000  sweep4 E= -0.600, M= -1.000

 sweep5 E= -0.600, M = -1.000  sweep6 E = 0.000, M = -0.500

 sweep7 E= 0.000, M =0.000  sweep8 E = - 0.600, M = 1.000

 sweep9 E= 0.00, M = 0.500  sweep10 E = -0.600, M = -1.000

Group 3

 sweep1 E = 0.000, M=0.000  sweep2 E= 0.000,M= 0.000

 sweep3 E = -0.600,M = - 1.000  sweep4 E= 0.000, M= 0.000

 sweep5 E= 0.000, M = 0.500  sweep6 E = -0.600, M = 1.000

 sweep7 E= 0.000, M =0.000  sweep8 E = - 0.600, M = -1.000

 sweep9 E= 0.00, M = 0.500  sweep10 E = 0.000, M = 0.000

Group 4

 sweep1 E = -0.600, M= 1.000  sweep2 E= -0.600,M= -1.000

 sweep3 E =- 0.600, M = 1.000  sweep4 E= 0.000, M= 0.500

 sweep5 E= -0.600, M = -1.000  sweep6 E = -0.600, M = -1.000

 sweep7 E= 0.000, M =0.500  sweep8 E = - 0.600, M = 1.000

 sweep9 E= =-0.600, M = 1.000  sweep10 E = -0.600, M = 1.000

Group 5

 sweep1 E = 0.000, M=0.000  sweep2 E= -0.600,M= -1.000

 sweep3 E = -0.600, M = - 1.000  sweep4 E= -0.600, M= 1.000

 sweep5 E= 0.000, M = 0.000  sweep6 E = 0.000, M = -0.500

 sweep7 E= -0.600, M =1.000  sweep8 E = - 0.000, M = 0.500

 sweep9 E= -0.600, M = -1.000  sweep10 E = 0.000, M = -0.500

Group 6

 sweep1 E = 0.000, M= -0.500  sweep2 E= 0.000,M= 0.000

 sweep3 E = -0.600, M = 1.000  sweep4 E= -0.600, M= - 1.000

 sweep5 E= -0.600, M = 1.000  sweep6 E = -0.600, M = 1.000

 sweep7 E= 0.000, M = 0.000  sweep8 E = - 0.600, M = 1.000

 sweep9 E= -0.600, M = 1.000  sweep10 E =- 0.600, M = 1.000

Group 7

 sweep1 E = 0.000, M= 0.000  sweep2 E= -0.600,M= 1.000

 sweep3 E =-0.000, M =-0.500  sweep4 E= 0.000, M= 0.000

 sweep5 E= -0.600, M = 1.000  sweep6 E = -0.600, M = 1.000

 sweep7 E= 0.000, M = 0.500  sweep8 E = 0.000, M = -0.500

 sweep9 E= -0.600, M = 1.000  sweep10 E =- 0.600, M = -1.000

Group 8

 sweep1 E = 0.000, M= 0.000  sweep2 E= 0.000,M= -0.500

 sweep3 E = -0.600, M = 1.000  sweep4 E= -0.600, M=1.000

 sweep5 E= -0.600, M = -1.000  sweep6 E = -0.600, M = 1.000


sweep7 E= 0.600, M =0.000


sweep8 E = -0.600, M = 1.000


sweep9 E= -0.600, M = 1.000


sweep10 E =- 0.600, M = -1.000

Group 9


sweep1 E = 0.000, M= 0.000


sweep2 E= 0.000,M= -0.000


sweep3 E = -0.600, M = -1.000


sweep4 E= -0.600, M= -1.000


sweep5 E= -0.600, M = 1.000


sweep6 E = -0.600, M = -1.000


sweep7 E= -0.600, M =-1.000


sweep8 E = 0.000, M = -0.500


sweep9 E= -0.000, M = -0.500


sweep10 E =- 0.000, M = 0.500

Group 10


sweep1 E = -0.600, M= 1.000


sweep2 E= 0.000,M= -0.500


sweep3 E = -0.600, M = 1.00


sweep4 E= -0.600, M= 1.000


sweep5 E= -0.600, M = 1.000


sweep6 E = -0.600, M = -1.000


sweep7 E= -0.600, M = -1.000


sweep8 E = -0.600, M = -1.000


sweep9 E= -0.600, M = -1.000


sweep10 E =- 0.600, M = 1.000

Figure 4.1 Spin –array in matrices form for 2 X 2 crystal lattice.

4.2.1 Energy E, Magnetization M, Susceptibility^{x}, Specific heat C_v for 2 X 2 Crystal lattice

These thermodynamic functions are the data generate for 2 X 2 lattice. They are the average values per group. The averages are over ten thermalization sweeps.

Table 4.1 Tabulated values for energy, magnetization, susceptibility and specific heat

Thermalization sweeps (in group)	Energy (E) (joules)	Magnetization (M) (amp/meter)	Susceptibility ^{x} (dimensionless)	Specific heat C_v joules/K/Kg
G1	-0.54	-0.25	3.45	0.13
G2	-0.36	-0.25	2	0.34
G3	-0.18	0	1.4	0.30
G4	-0.48	0.3	3.04	0.23
G5	-0.3	-0.15	2.21	0.36
G6	-0.42	0.45	2.09	0.30
G7	-0.3	0.25	2.05	0.36
G8	-0.36	0.25	2.65	0.63
G9	-0.3	-0.15	2.21	0.36
G10	-0.45	0.15	3.21	0.23

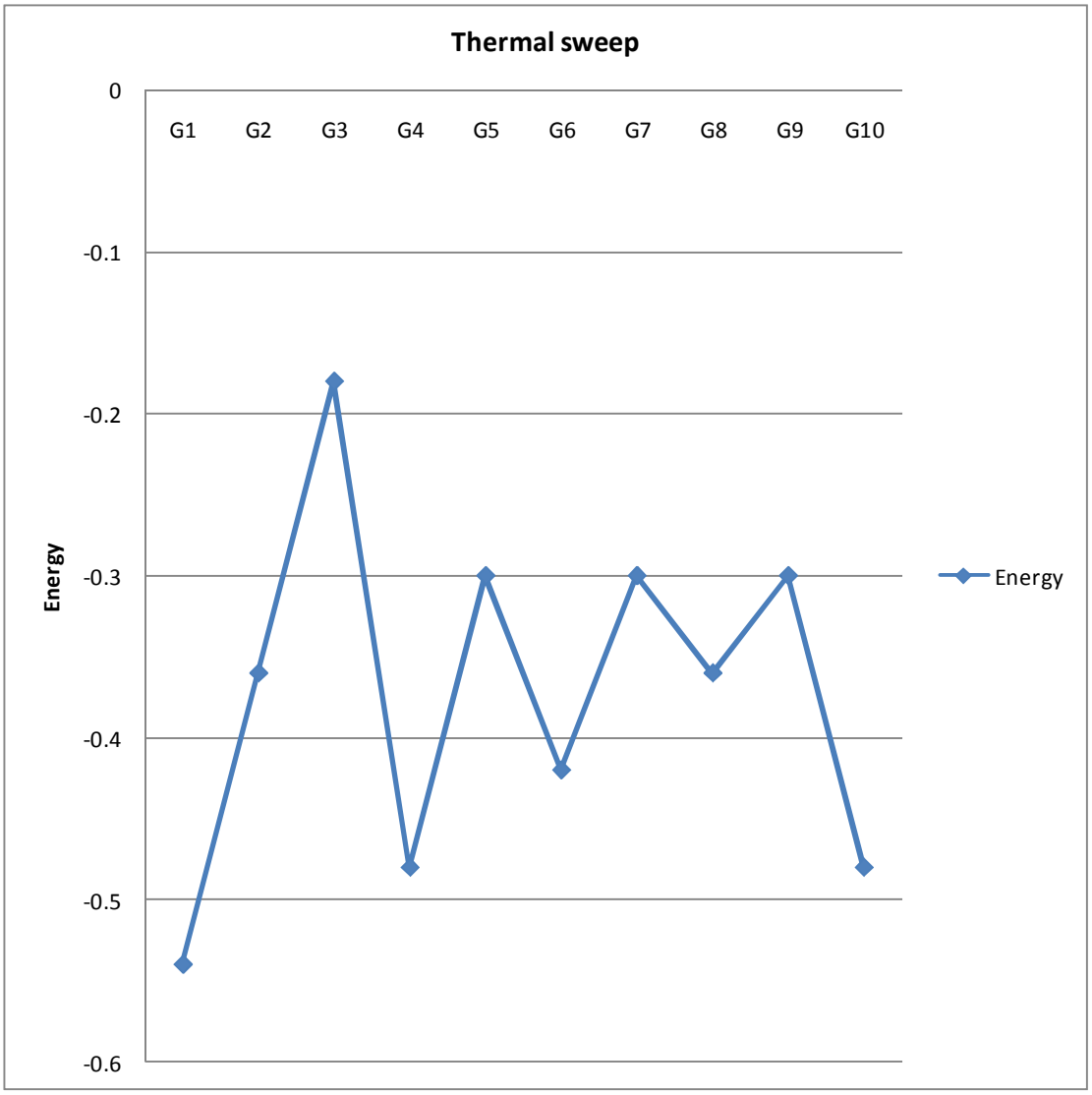


Figure 4.2 Energy as function of thermalization sweep of 2 by 2 crystal lattice.

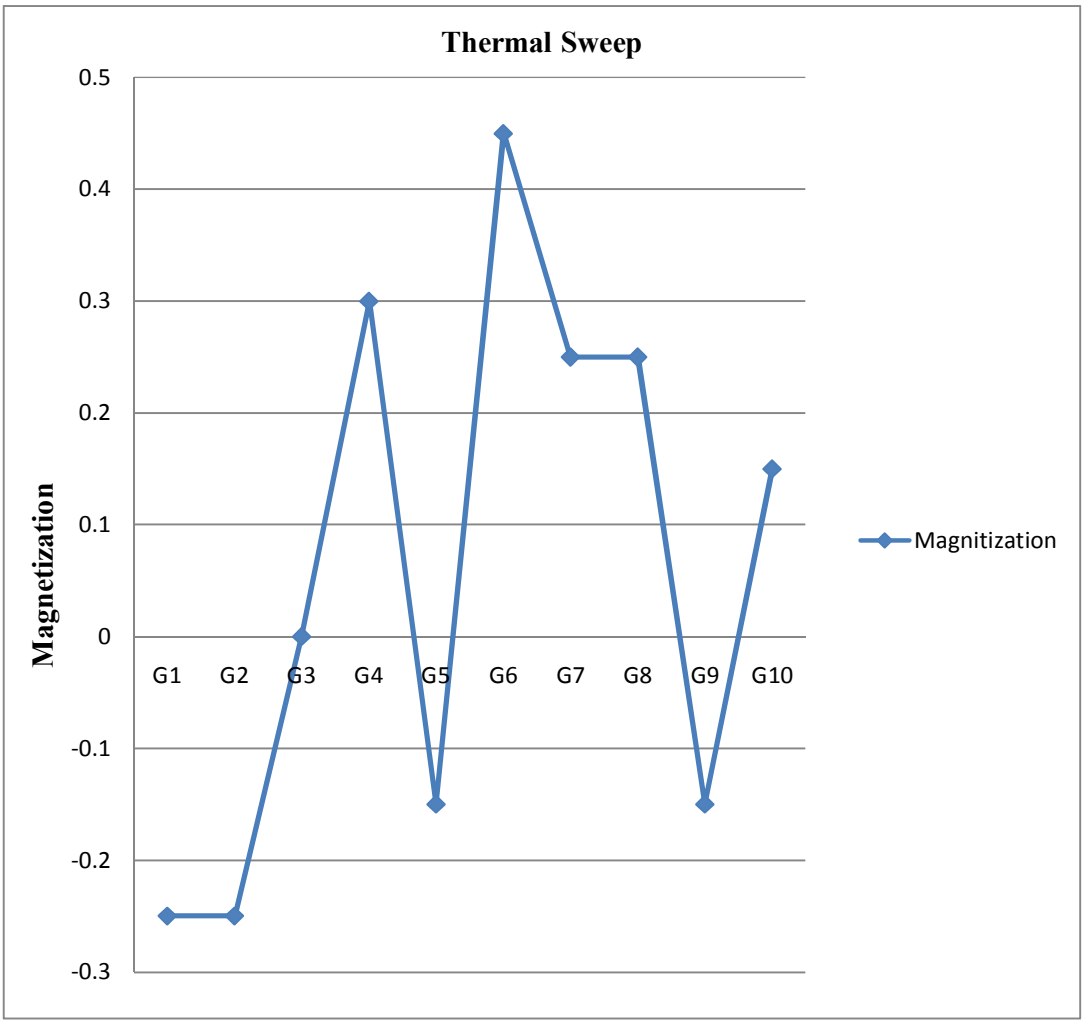


Figure 4.3 Magnetization as function of thermalization sweep of 2 by 2 crystal lattice.

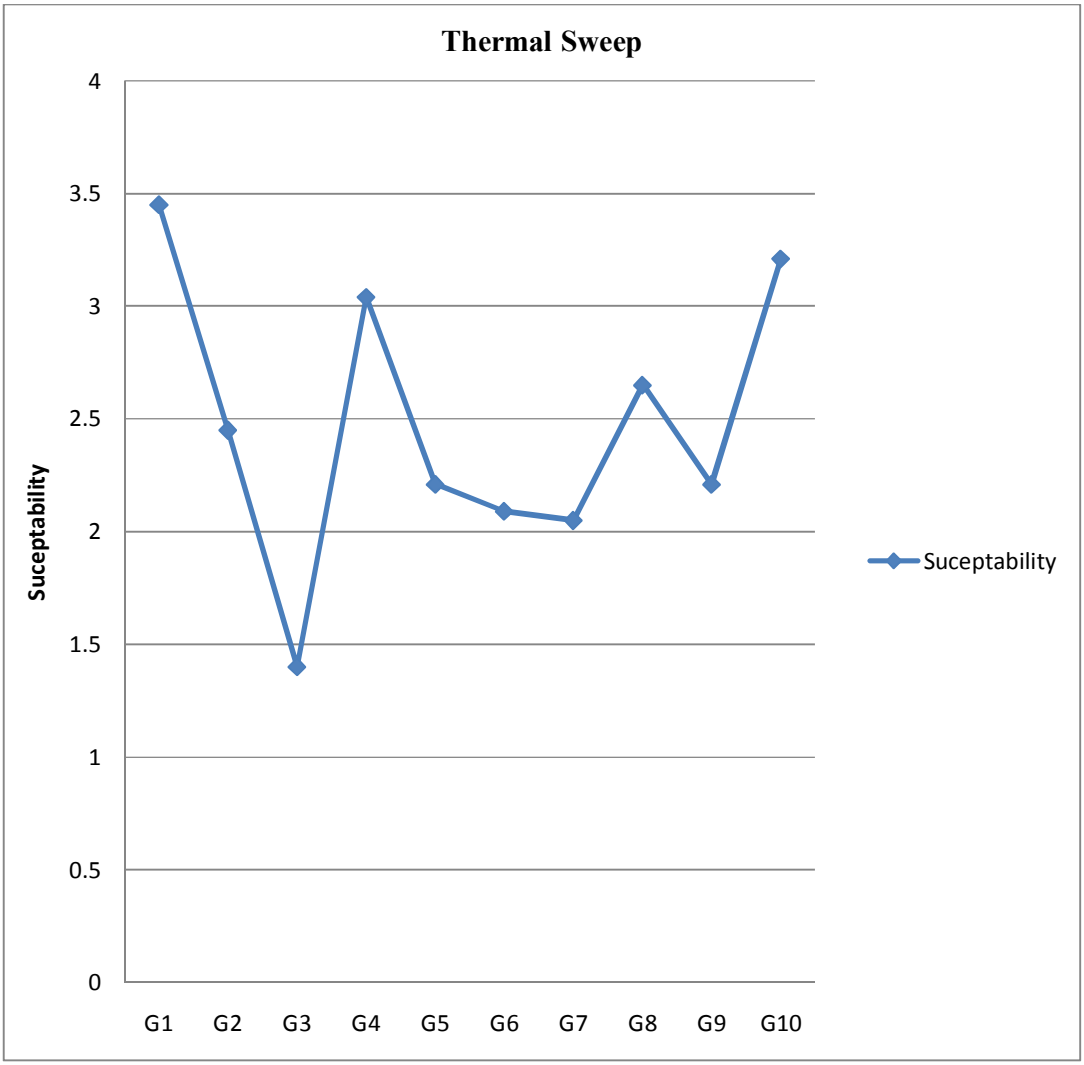


Figure 4.4 Susceptibility as a function of thermalization sweep of 2 by 2 crystal lattice.

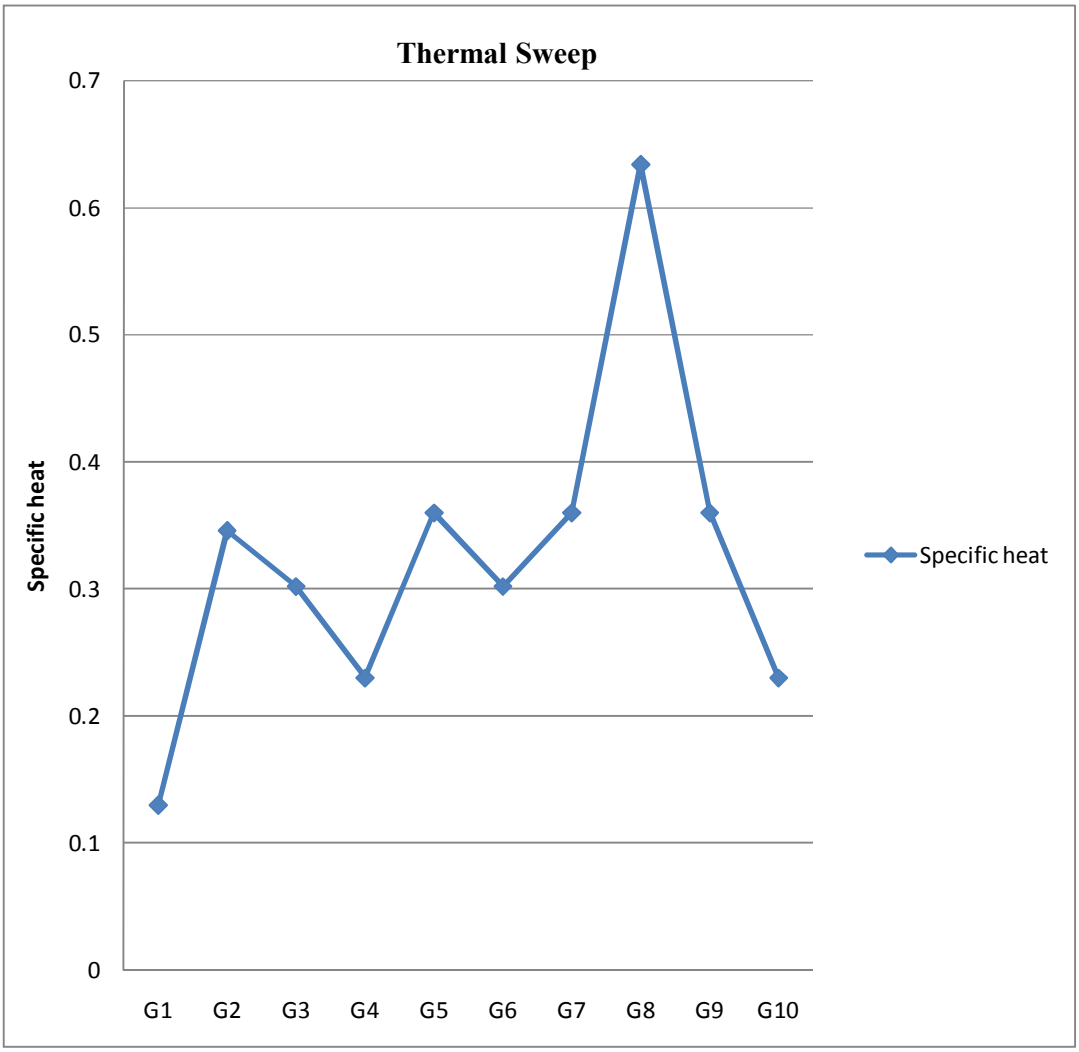
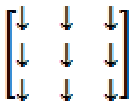
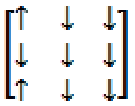


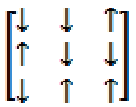
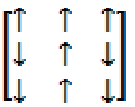
Figure 4.5 Specific heat as a function of thermalization sweep of 2 by 2 crystal lattice.

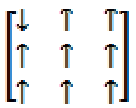
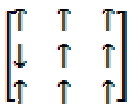
4.3 SIMULATION OF SPIN ALIGNMENT FOR 3 X 3 CRYSTAL LATTICE.

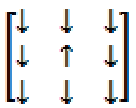
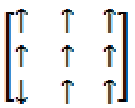
Below is the spin –array display that was obtained on running the code for 3 x3 lattice structure under the condition of magnetic field of 0.0001 KT , interacting strength of 0.300 KT ten thermalization sweeps and ten groups respectively. The spin snapshot is presented in matrices in order to obtain accurate and precise result.

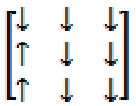
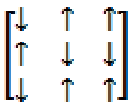
Group 1

 sweep1 E= -0.600, M= -1.000  sweep2 E= -0.200, M= 0.556

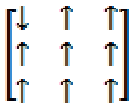
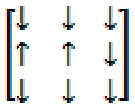
 sweep3 E= 0.200, M= -0.111  sweep4 E= -0.067,M= 0.111

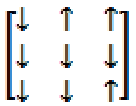
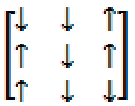
 sweep5 E= -0.333, M = 0.778  sweep6 E= -0.333, M= 0.778

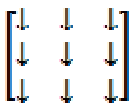
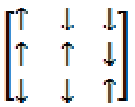
 sweep7 E=-0.333 , M= -0.778  sweep8 E=-0.333,M= 0.778

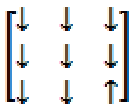
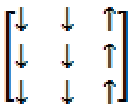
 sweep9 E= -0.200, M=-0.556  sweep10 E=0.200,M= 0.111

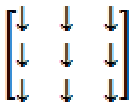
Group 2

 sweep1 E= -0.333, M = 0.778  sweep2 E= -0.200, M = 0.556

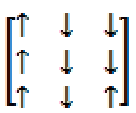
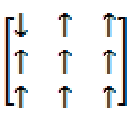
 sweep3 E= -0.067, M= -0.333  sweep4 E= 0.067, M= - 0.111

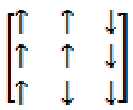
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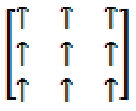
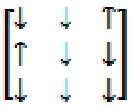
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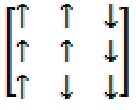
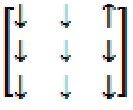
 sweep9 E= -0.600, M=-1.000  sweep10 E= -0.200, M= -.556

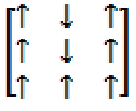
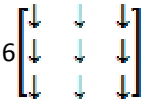
Group 3

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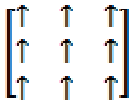
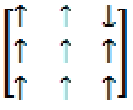
 sweep3 E= -0.600, M=1.000  sweep4 E= -0.067, M= 0.111

 sweep5 E= -0.600, M=1.000  sweep6 E= -0.067, M= -0.556

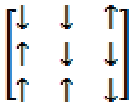
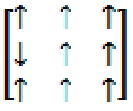
 sweep7 E= -0.067, M=0.111  sweep8 E= -0.600, M= -1.000

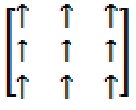
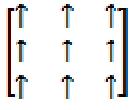
 sweep9 E= -0.200, M= 0.556  sweep10 E= -0.600, M= -1.000

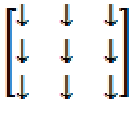
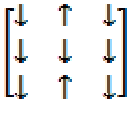
Group 4

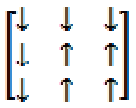
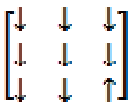
 sweep1 E= -0.600, M=1.000  sweep2 E= -.333,M=

0.778

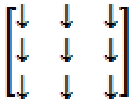
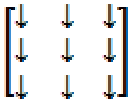
 sweep3 E=0.200, M= -0.111  sweep4 E= -0.000,M= 3.000

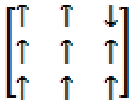
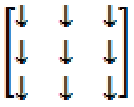
 sweep5 E= -0.600, M= 1.000  sweep6 E= -0.600, M= 1.000

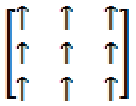
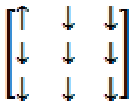
 sweep7 E= -0.600, M= -1.000  sweep8 E= -0.200, M= -0.556

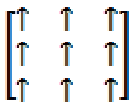
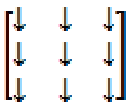
 sweep9 E= 0.067, M= -0.111  sweep10 E= -0.333, M= -0.778

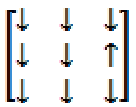
Group 5

 sweep1 E= - 0.600, M= -1.000  sweep2 E= -0.600, M= -1.000

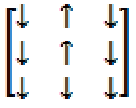
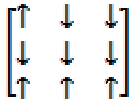
 sweep3 E= -0.333, M=0.778  sweep4 E= -0.600, M= -1.000

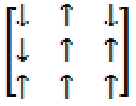
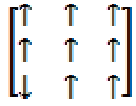
 sweep5 E= -0.600, M=1.000  sweep6 E= -0.333, M= -0.778

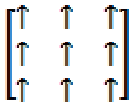
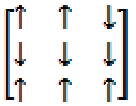
 sweep7 E= -0.600, M=1.000  sweep8 E= -0.600, M= -1.000

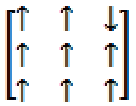
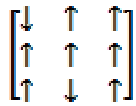
 sweep9 E= -0.333, M=-0.778  sweep10 E= -0.200, M= 0.556

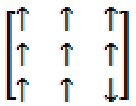
Group 6

 sweep1 E= -0.200, M= -0.556  sweep2 E= -0.067, M= -0.111

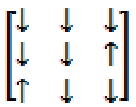
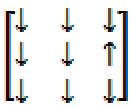
 sweep3 E= -0.067 M= 0.333  sweep4 E= -0.333,M= 0.778

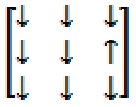
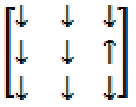
 sweep5 E= -0.600, M=1.000  sweep6 E= -0.067, M= 0.111

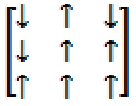
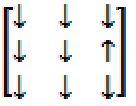
 sweep7 E= -0.333, M= 0.778  sweep8 E= -0.067, M= 0.556

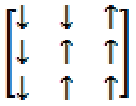
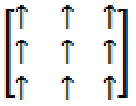
 sweep9 E= -0.333, M= 0.778  sweep10 E= --0.333, M= 0.778

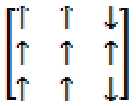
Group 7

 sweep1 E= -0.333, M= -0.778  sweep2 E= -0.600, M= -1.000

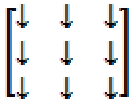
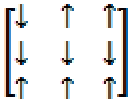
 sweep3 E= -0.600, M= -1.000  sweep4 E= -0.600, M= -1.000

 sweep5 E= -0.067, M=0.333  sweep6 E= -0.600, M= -1.000

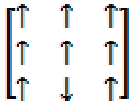
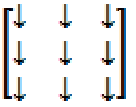
 sweep7 E= -0.607, M= -0.111  sweep8 E= -0.600, M= 1.000

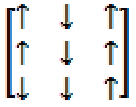
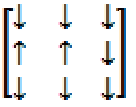
 sweep9 E= -0.200, M= -0.556  sweep10 E= -0.067, M= -0.111

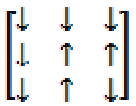
Group 8

 sweep1 E= -0.600, M= -1.000  sweep2 E= -0.067,M= 0.111

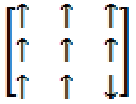
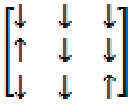
 sweep3 E= -0.600, M= 1.000  sweep4 E= -0.600, M= 1.000

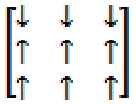
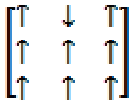
 sweep5 E= -0.333, M=0.778  sweep6 E= -0.600, M= -1.000

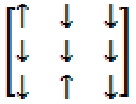
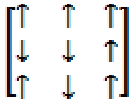
 sweep7 E= -0.067, M=0.111  sweep8 E= -0.200, M= -0.556

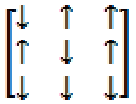
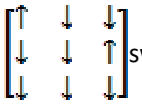
 sweep9 E=- 0.067, M= -0.333  sweep10 E= - 0.333,M= 0.778

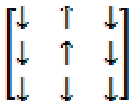
Group 9

 sweep1 E=-0.333, M=0.778  sweep2 E= -0.067, M= 0.556

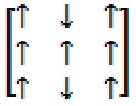
 sweep3 E= -0.200, M=0.333  sweep4 E= -0.333 M= 0.778

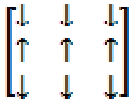
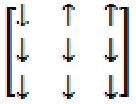
 sweep5 E=0.067, M= -0.556  sweep6 E= -0.067,M= 0.333

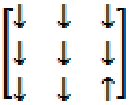
 sweep7 E=0.067, M= 0.111  sweep8 E= -0.067, M= -0.556

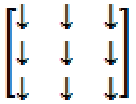
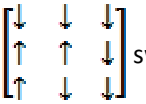
 sweep9 E= -0.200, M= -0.556  sweep10 E= -0.200, M= -0.556

Group 10

 sweep1 E= -0.200, M= -0.556  sweep2 E= -0.333, M= 0.778

 sweep3 E= -0.200, M= 0.333  sweep4 E= -0.200, M= -0.556

 sweep5 E= -0.333, M=0.778  sweep6 E= -0.333, M= -0.778

 sweep7 E= -0.600, M= - 1.000  sweep8 E= -0.200, M= -0.556

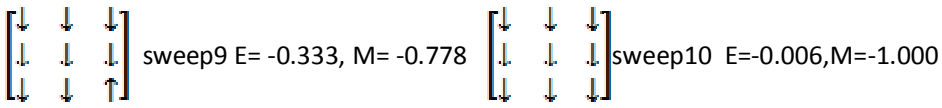


Figure 4.6 Spin –array in matrices form for 3 X 3 crystal lattice.

4.3.1 Energy E, Magnetization M, Susceptibility ^{x}, Specific heat C_v for 3 X 3 Crystal lattice

These thermodynamic functions are the data generate for 3 X 3 lattice. They are the average values per group. The averages are over ten thermalization sweeps.

Table 4.2 Tabulated values for energy magnetization, susceptibility and specific heat.

Thermalizaation sweep (in group)	Energy E (joules)	Magnetization M (amp/m)	Susceptibility ^{x} (dimensionless)	Specific heat C_v Joule/K/Kg
G1	-0.200	0.044	3.649	0.512
G2	-0.22	0.400	2.227	0.538
G3	-0.32	-0.089	4.662	0.526
G4	-0.347	0.20	5.173	0.59
G5	-0.48	-0.22	6.867	0.206
G6	-0.24	0.444	1.978	0.258
G7	-0.36	-0.311	4.572	0.602
G8	-0.347	0.089	5.018	0.462
G9	-0.147	-0.067	2.649	0.134
G10	-0.349	0.133	4.84	0.302

As it appeared in the 2 X 2 lattice, magnetization has six positive values and four negative values as well.

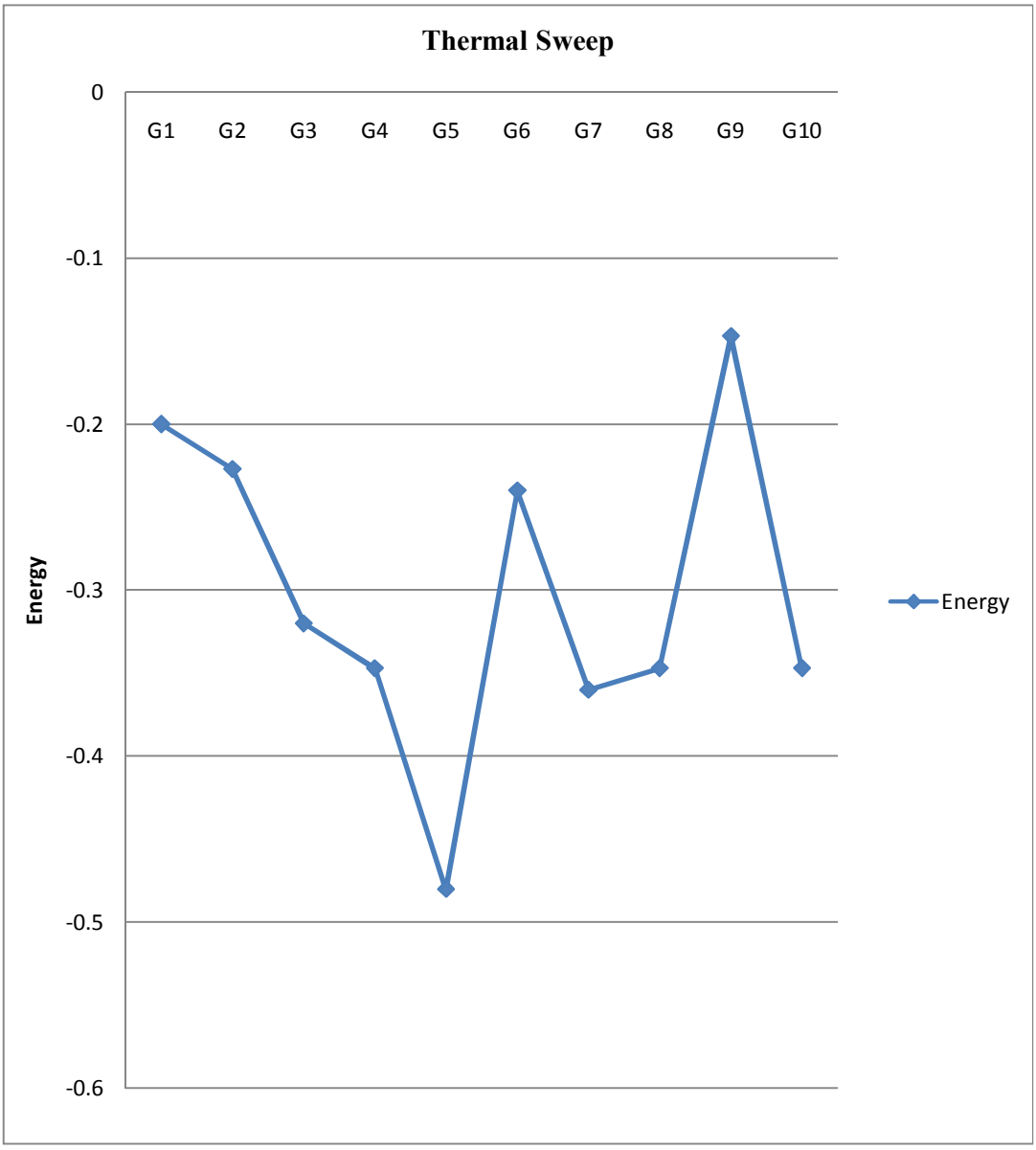


Figure 4.7 Energy as a function of thermalization sweep of 3 by 3 crystal lattice.

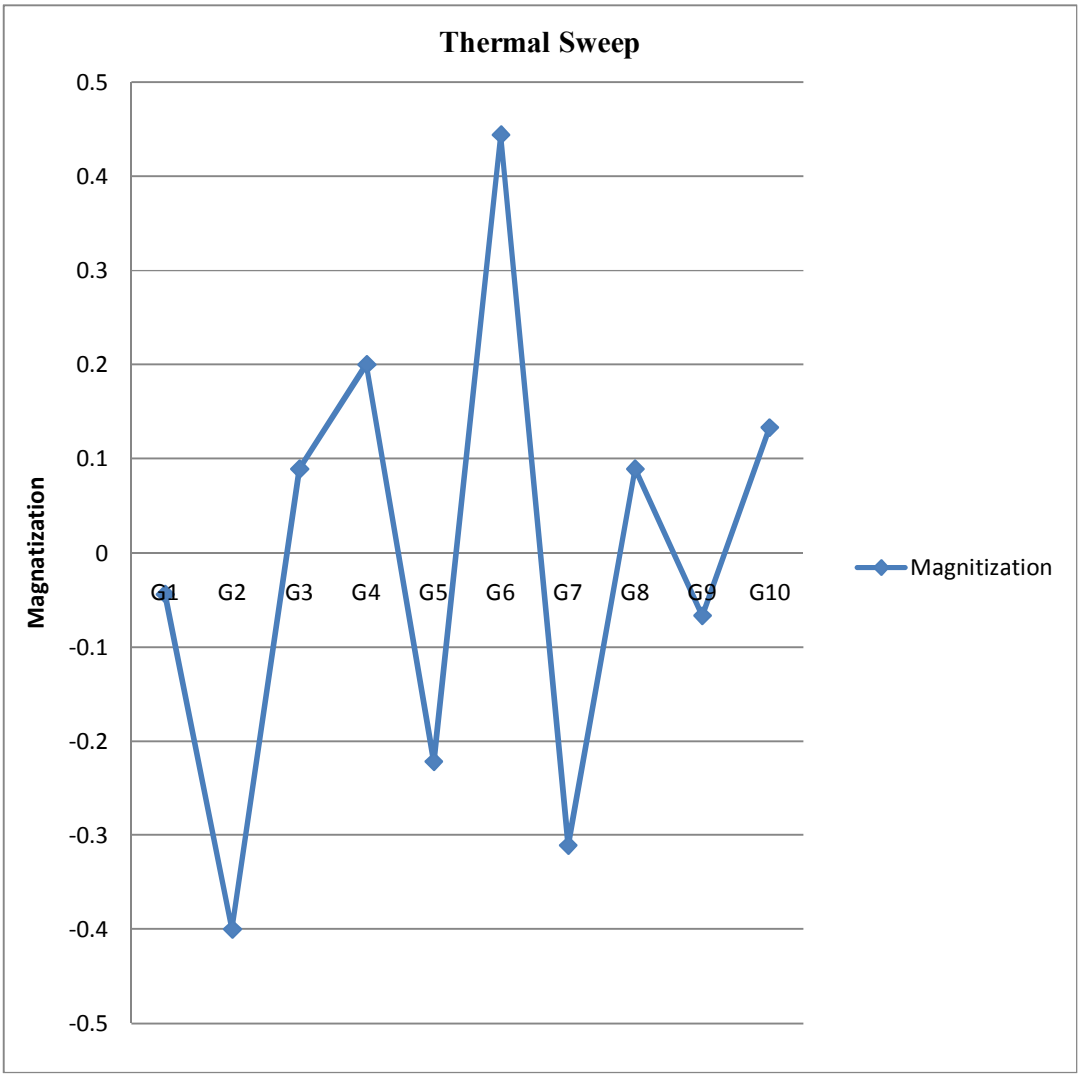


Figure 4.8 Magnetization as a function of thermalization sweep of 3 by 3 crystal lattice.

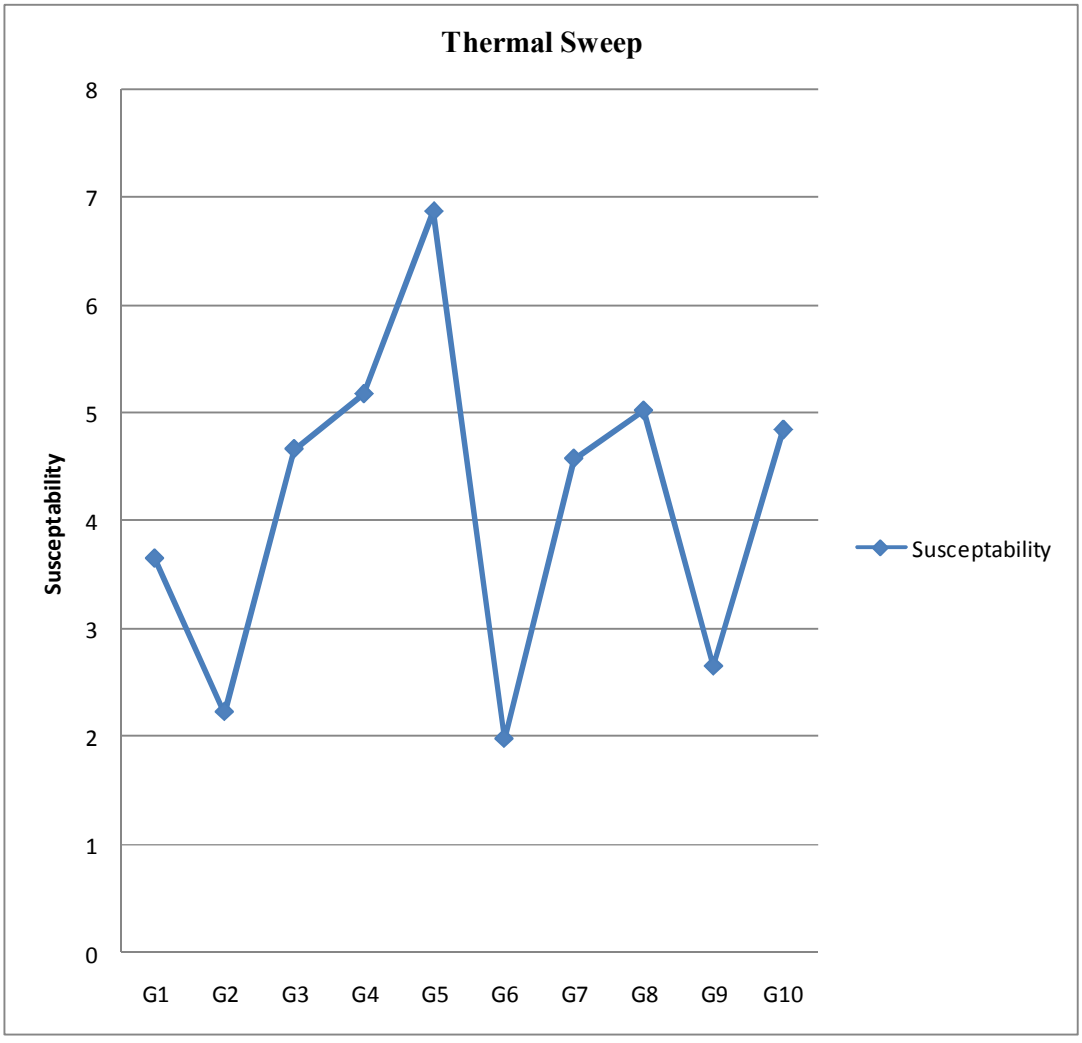


Figure 4.9 Susceptibility as a function of thermalization sweep of 3 by 3 crystal lattice.

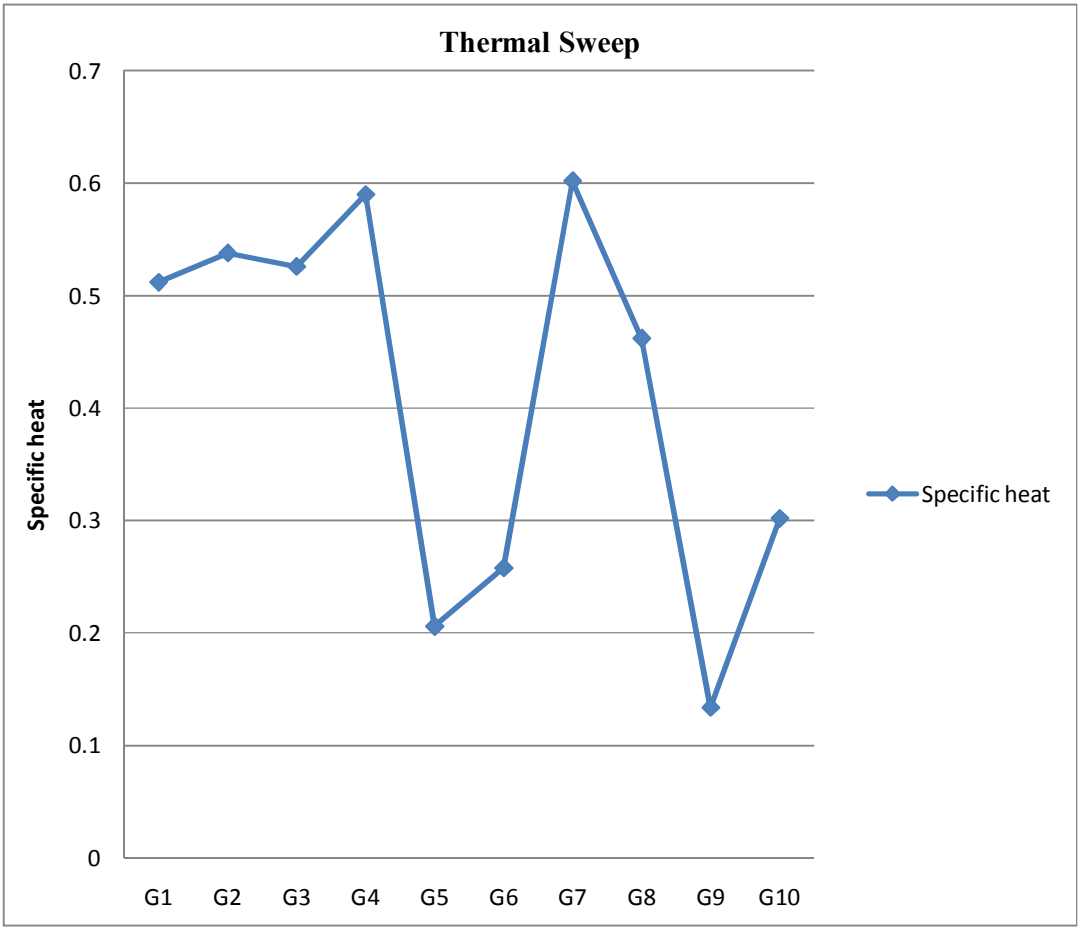
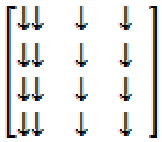
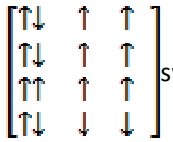


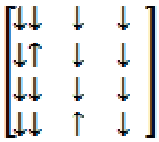
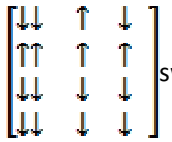
Figure 4.9 Specific heat as a function of thermalization sweep of 3 by 3 crystal lattice.

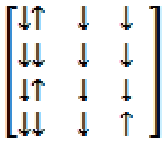
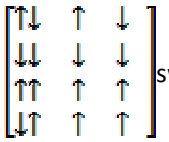
4.4 SIMULATION OF SPIN ALIGNMENT FOR 4 X 4 CRYSTAL LATTICE.

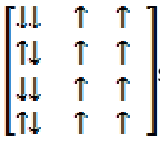
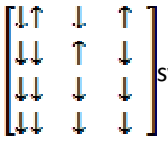
Below is the spin –array display that was obtained on running the code foe 4 x 4 lattice structure under the condition of magnetic field of 0.0001 kT , interacting strength of 0.300 kT ten thermalization sweeps and ten groups respectively. The spin snapshot is presented in matrices in order to obtain accurate and precise result.

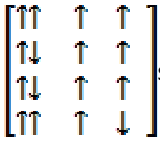
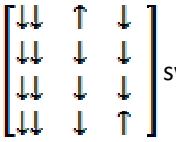
Group 1


sweep1 E= -0.600,M = -1.000

sweep2 E= -0.150,M = 0.375

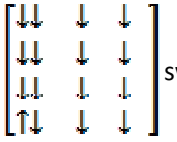
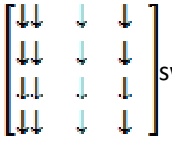

sweep3E= -0.300,M = -0.750

sweep4 E=-0.225,M = -0.375

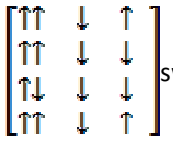
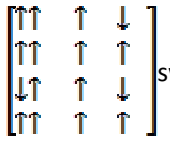

sweep5 E= -0.150,M = -0.625

sweep6 E= 0.000,M = 0.125

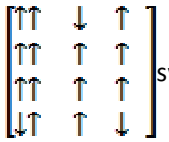
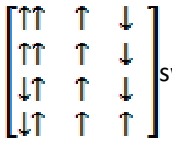

sweep7 E= -0.150,M = 0.250

sweep8 E= -0.150,M = -0.625

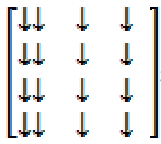
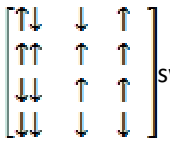

sweep9 E=-0.225,M = 0.625

sweep10 E= -0.300,M = -0.750

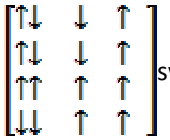
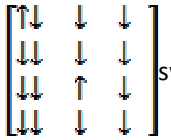
Group 2


sweep1 E= -0.450,M = -0.875

sweep2 E= -0.600,M = -1.000

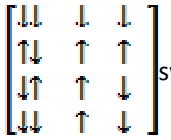
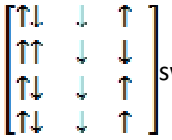

sweep3 E= -0.150,M = 0.125

sweep4 E= -0.225,M = 0.625


sweep5 E= -0.225,M = 0.625

sweep6 E= -0.150,M = 0.375

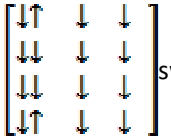
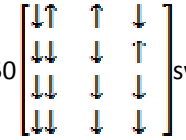

sweep7 E= -0.600,M =-1.000

sweep8 E= -0.150,M = 0.000


sweep9E=-0.150,M = 0.250

sweep10 E=-0.450,M = -0.875

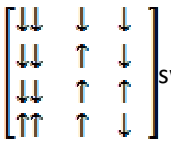
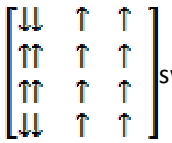
Group3

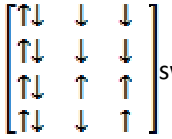
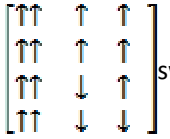

sweep1E= -0.075,M = -0.250

sweep2 E= -0.150,M =

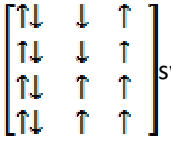
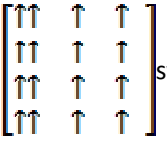
0.000


sweep3E= -0.375,M= -0.750

sweep4 E= -0.225,M =

-0.625

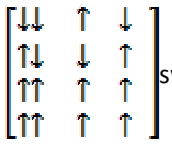
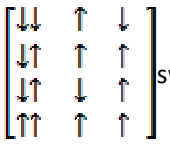

sweep5 E= -0.075,M= -0.250

sweep6 E= -0.300,M = 0.500


sweep7 E= -0.150,M =-0.125

sweep8 E= -0.300,M = 0.625

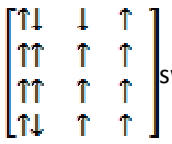
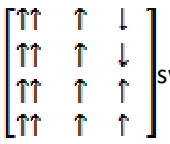

sweep9E= -0.225,M = 0.250

sweep10 E= -0.600,M =

1.000

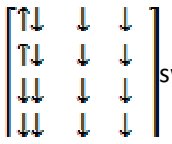
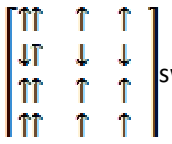
Group 4


sweep1 E= -0.150,M = 0.375

sweep2 E= 0.000,M =

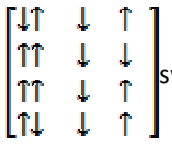
0.250


sweep3 E= -0.300,M = 0.625

sweep4 E= -0.375,M =

0.750

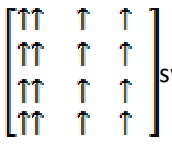
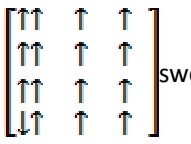

sweep5E= -0.375,M = -0.750

sweep6 E= -0.300,M =

0.625


sweep7 E= -0.000,M = 0.125

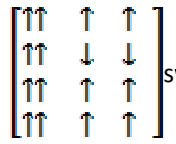
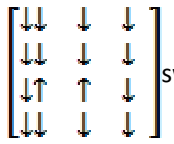
sweep8 E= -0.225,M =

0.625

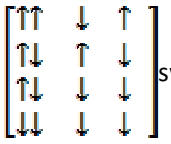
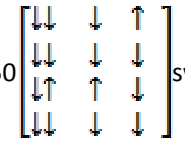

sweep9E= -0.600,M =1.000

sweep10 E= -0.450,M =

0.875

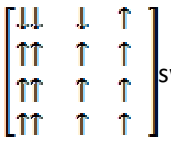
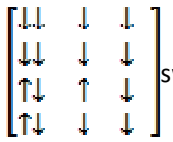
Group5


sweep1E= -0.375,M = 0.750

sweep2 E= -0.450,M =

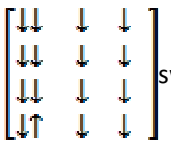
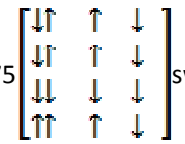
-0.875


sweep3E= -0.000,M = -0.250

sweep4E= -0.450,M =

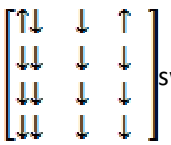
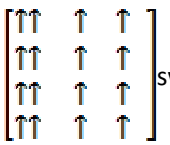
-0.875


sweep5 E=-0.300,M = 0.625

sweep6 E= -0.375,M =

-0.750

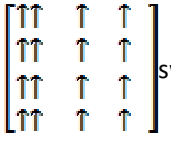
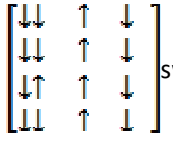

sweep7 E= -0.450,M = -0.875

sweep8 E= -0.075,M =

0.000

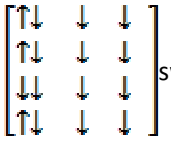
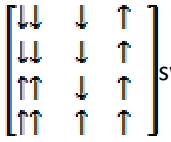

sweep9 E=-0.375,M =-0.750

sweep10 E= -0.600,M =

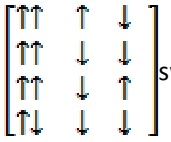
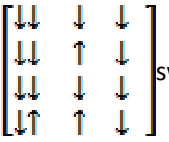
1.000

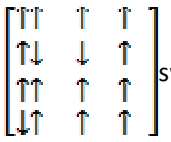
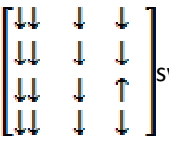
Group 6

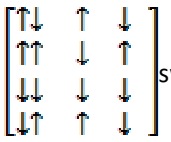
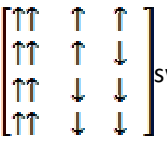

sweep1 E=-0.600,M = 1.000

sweep1 E= -0.225,M =

-0.375

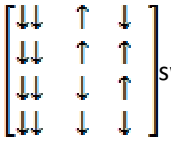
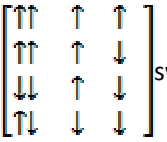

sweep3 E=-0.300,M= -0.625

sweep4 E= -0.150,M = 0.125

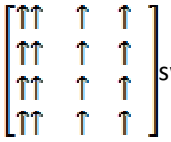

sweep5 E=-0.075,M =0.125

sweep6 E= -0.375,M = -0.750


sweep7 E=-0.225,M = 0.625

sweep8 E= -0.450,M = -0.875

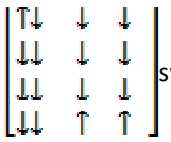
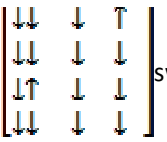

sweep9 E=- 0.075,M=-0.125

sweep10 E= -0.225,M = 0.375

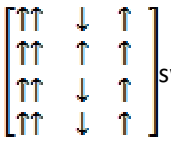
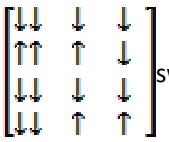
Group 7

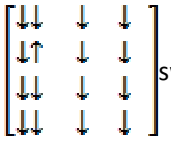
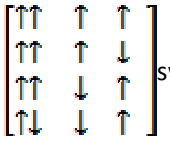

sweep1 E=-0.225,M =- 0.500

sweep2 E= -0.075,M = 0.125


sweep3 E=-0.600,M = 1.000

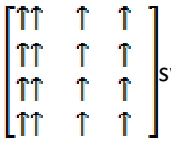
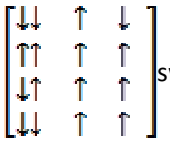
sweep4 E= -0.600,M = 1.000

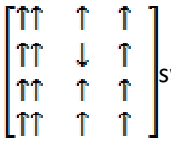

sweep5E=-0.225,M =-0.625

sweep6 E= -0.300,M = -0.750


sweep7 E=-0.225,M = 0.625

sweep8 E= -0.150,M = -0.375

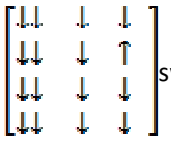
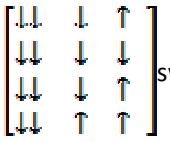

sweep9 E=-0.450,M=-0.875

sweep10 E= -0.150,M = 0.500

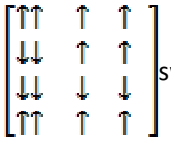
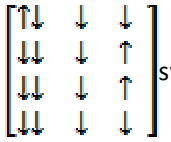
Group 8

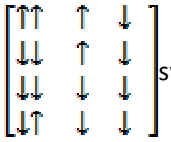
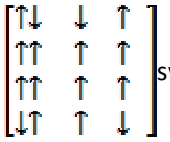

sweep1 E= -0.600,M = 1.000

sweep2 E= -0.150,M = 0.250


sweep3 E= -0.450,M = 0.875

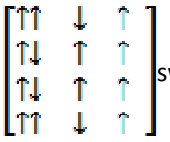
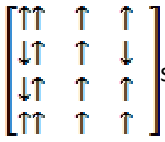
sweep4 E= -0.150,M = 0.500

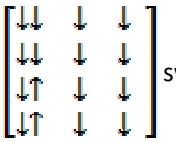
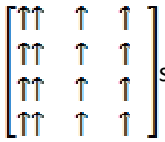

sweep5 E=-0.450,M=-0.875

sweep6 E= -0.225,M = -0.500

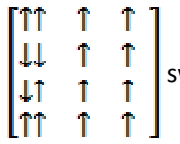
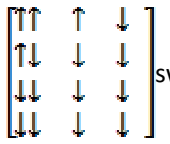

sweep7 E=-0.225,M=0.250

sweep8 E= -0.-225,M = -0.625


sweep9 E=-0.150,M=-0.375

sweep10 E= -0.150,M = 0.500

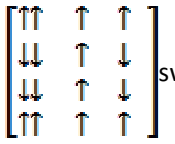
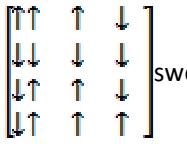
Group 9

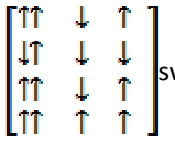
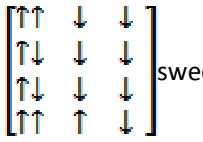

sweep1 E=-0.150,M = 0.500

sweep2 E= -0.300,M = 0.625


sweep3E=-0.375,M=-0.750

sweep4 E= -0.600,M = 1.000

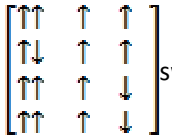
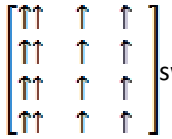
 sweep5E=-0.300,M=0.625  sweep6E=-0.225,M= -

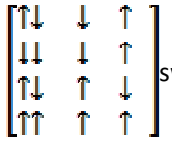
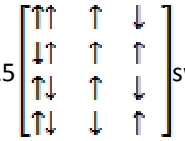
0.500

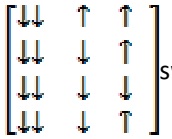
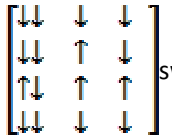
 sweep7E=-0.225,M=0.250  sweep8 E= -0.075,M = 0.000

 sweep9 E=-0.150,M=0.375  sweep10 E=-0.150,M = -0.125

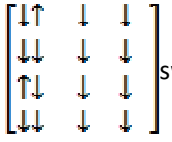
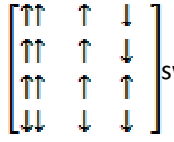
Group 10

 sweep1 E= -0.225,M = 0.625  sweep2 E= -0.450,M = 0.875

 sweep3 E= -0.000,M = 0.125  sweep4 E= -0.150,M = 0.500

 sweep5E=-0.225,M =-0.500  sweep6E= -0.225,M = -

0.500

 sweep7E= -0.375,M = -0.750  sweep8 E= -0.225,M = 0.250

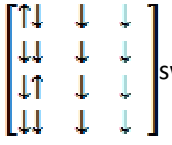
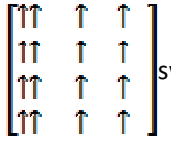
 sweep9E=-0.300,M=0.750  sweep10 E=-0.600, M= 1.000

Figure 4.11 Spin –array in matrices form for 4 X 4 crystal lattice.

4.4.1 Energy E, Magnetization M, Susceptibility ^{x}, Specific heat Cv for 4 X4 Crystal lattice

These thermodynamic functions are the data generate for 4 X 4 lattices. They are the average values per group. The averages are over ten thermalization sweeps.

Table 4.3 Tabulated values for energy, magnetization, susceptibility and specific heat

Thermalization sweep(in groups)	Energy E (joules)	Magnetization M (amp/m)	Susceptibility ^{x} (dimensionless)	Specific heat (joule/K/kg)
G1	-0.22	-0.27	4.64	0.36
G2	-0.315	-0.17	6.76	0.51
G3	-0.248	0.03	4.45	0.36
G4	-0.278	0.45	3.61	0.52
G5	-0.345	-0.2	8.06	0.47
G6	-0.255	-0.05	5.46	0.52
G7	-0.3	0.01	7.62	0.50
G8	-0.27	0.1	6.14	0.37
G9	-0.25	0.2	4.26	0.32
G10	-0.278	0.23	5.67	0.37

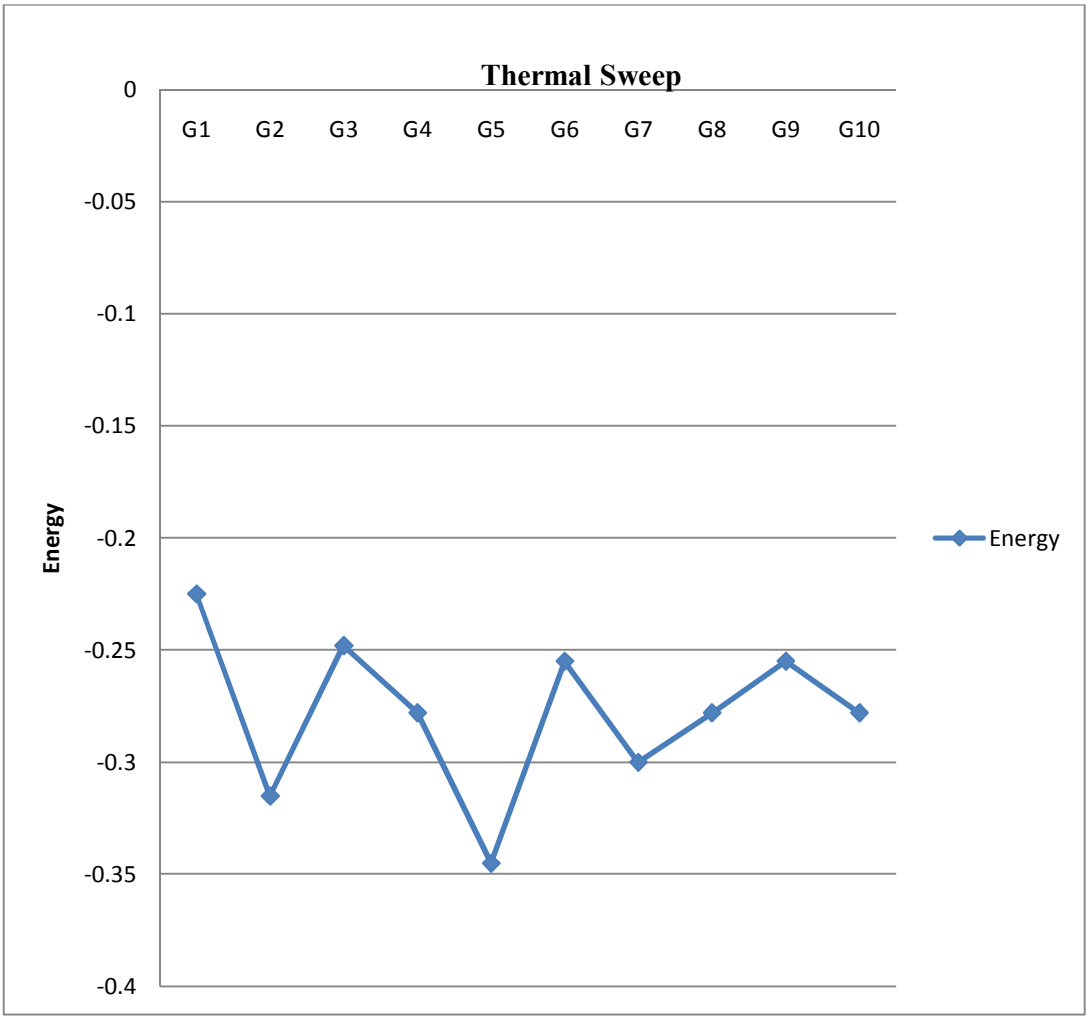


Figure 4.12 Energy as a function of thermalization sweep of 4 by 4 crystal lattice.

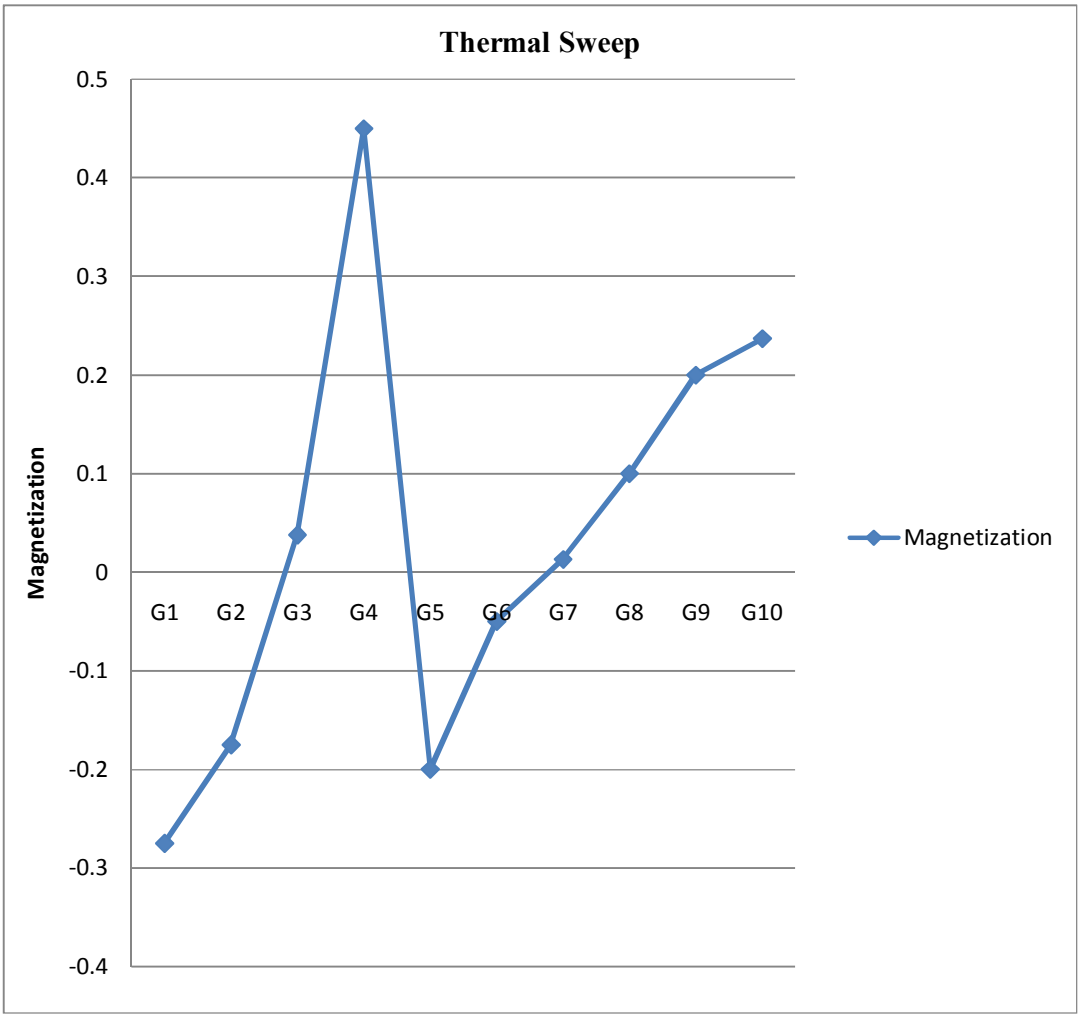


Figure 4.13 Magnetization as a function of thermalization sweep of 4 by 4 crystal lattice.

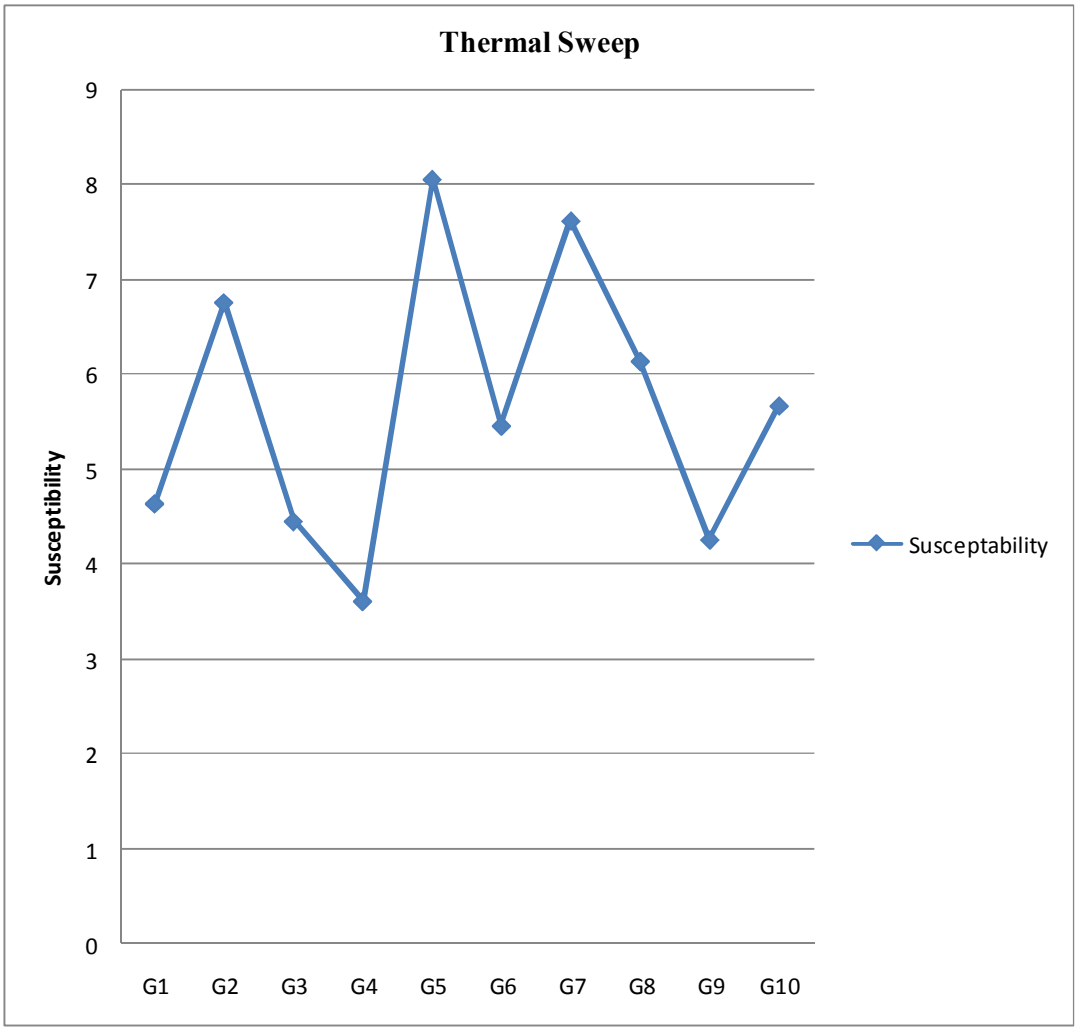
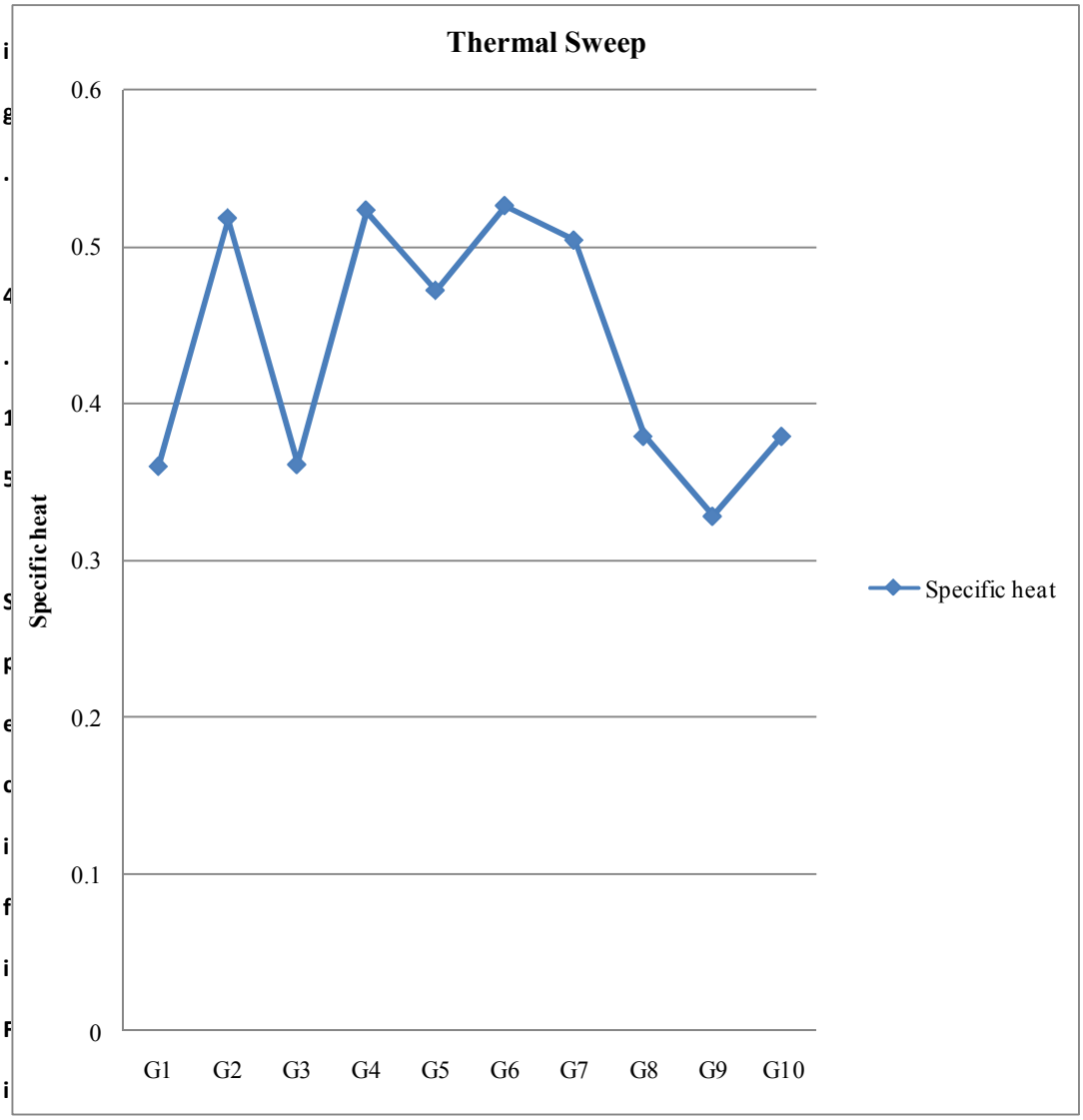


Figure 4.14 Susceptibility as a function of thermalization sweep of 4 by 4 Crystal lattice.

Fig. 4.15 Specific

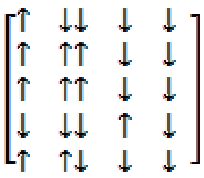
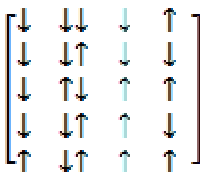


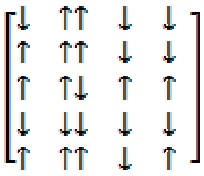
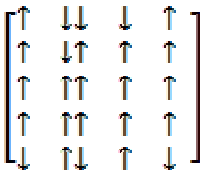
FFigure 4.15 specific heat as a function of thermalization sweep of 4 by 4 crystal lattice.

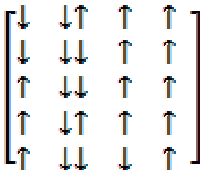
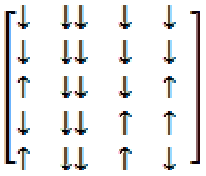
4.5 SIMULATION OF SPIN ALIGNMENT FOR 5 X 5 CRYSTAL LATTICE.

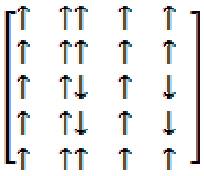
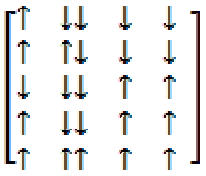
Below is the spin –array display that was obtained on running the code for 5 x 5 lattice structure under the condition of magnetic field of 0.0001 kT , interacting strength of 0.300 kT ten thermalization sweeps and ten groups respectively. The spin snapshot is presented in matrices in order to obtained accurate and precise result.

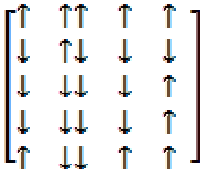
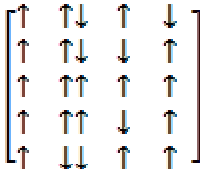
Group 1


sweep1 E=-0.120,M=-0.280

sweep2E= 0.024,M= -0.120

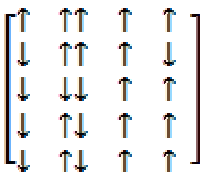
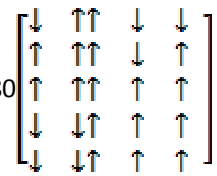

sweep3 E= -0.072, M= 0.040

sweep4 E= -0.168, M= -0.040

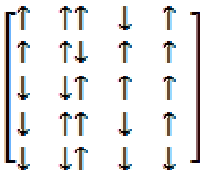
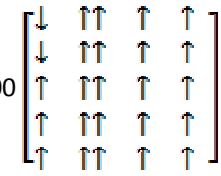

sweep5 E= -0.168, M= 0.120

sweep6 E= -0.216, M= -0.520

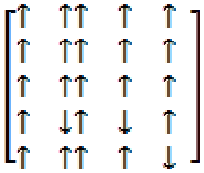
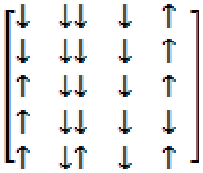

sweep7 E= -0.312, M= 0.680

sweep8 E= -0.120, M= 0.040

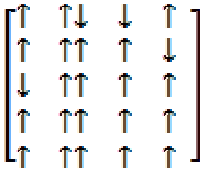
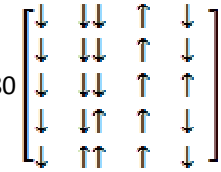

sweep9 E= -0.168, M= -0.120

sweep10 E -0.216, M= 0.520

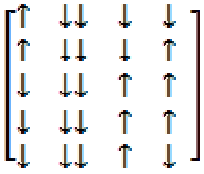
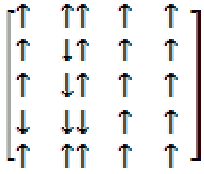
Group 2


sweep1 E= -0.120, M= 0.280

sweep2 E= -0.216, M= 0.360

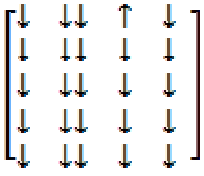
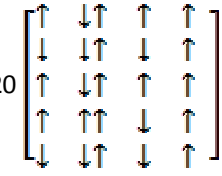

sweep3 E= -0.024, M= 0.200

sweep4 E= -0.000, M= -0.000

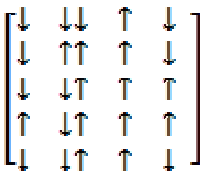

sweep5 E=-0.312, M= 0.760

sweep6 E=-0.168, M= -0.360


sweep7 E= -0.264, M= 0.680

sweep8 E= -0.216, M= -0.280

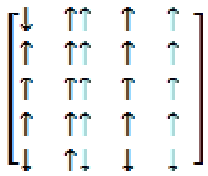

sweep9 E= -0.216, M= -0.360

sweep10 E=-0.312,M= 0.600

Group 3

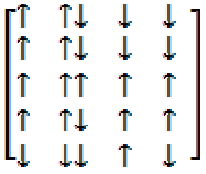

sweep1 E= -0.504 M= -0.920

sweep2 E= -0.024, M= -0.28



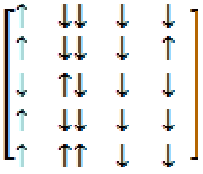
sweep3 E= -0.168, M= 0.040



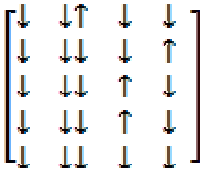
sweep4 E= -0.312, M= -0.600



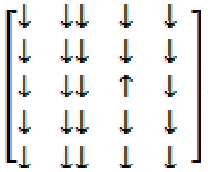
sweep5 E= -0.168 M= 0.120



sweep6 E= -0.072, M= -0.280

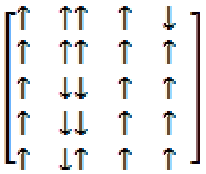


sweep7 E= -0.264 M= -0.680

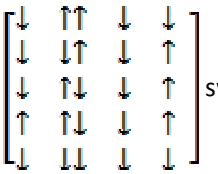


sweep8 E= -0.504, M= -0.920

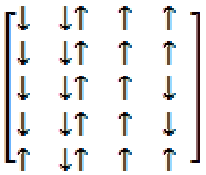
Group 4



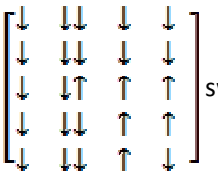
sweep1 E= -0.264, M= 0.520



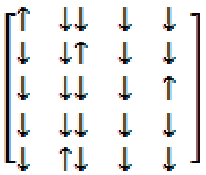
sweep2 E= -0.072, M= -0.280



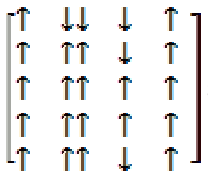
sweep3 E= -0.264, M= 0.120



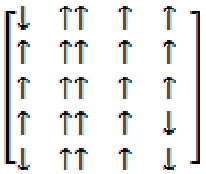
sweep4 E= -0.312, M= -0.520



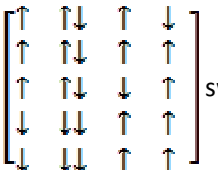
sweep5 E= -0.264, M= -0.680



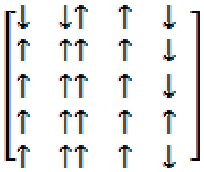
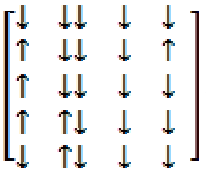
sweep6 E= -0.312, M= 0.600



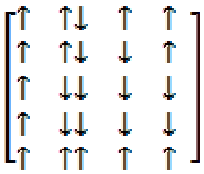
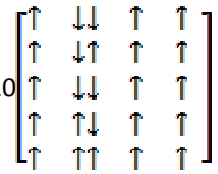
sweep7 E= -0.360, M= 0.680

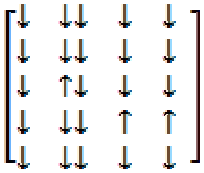
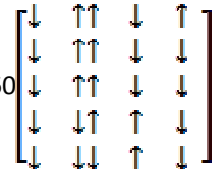


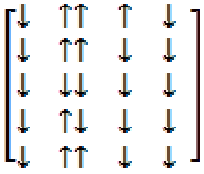
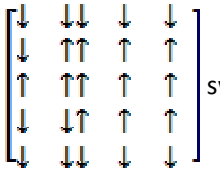
sweep8 E= -0.216, M= 0.200

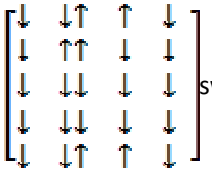
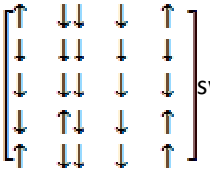

sweep9 E= -0.264,M= 0.520

sweep10 E=-0.264, M= -0.520

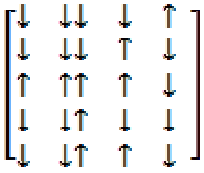
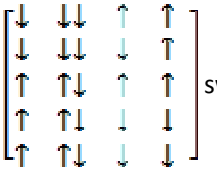
Group 5


sweep1 E= -0.216, M= -0.120

sweep2 E= -0.264, M= 0.520

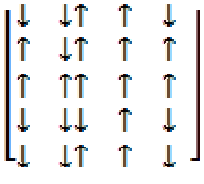
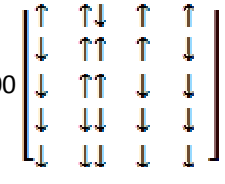

sweep3 E= -0.360, M= -0.760

sweep4 E= -0.120, M= -0.200

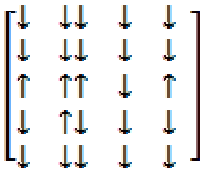
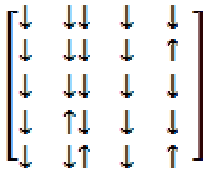

sweep5 E -0.216, M= -0.280

sweep6 E= -0.264, M= -0.040

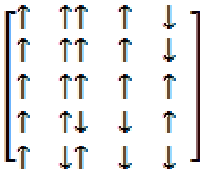
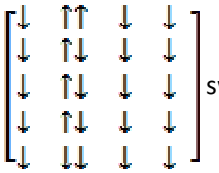

sweep7E=-0.312M=-0.520

sweep8E=-0.264,M=-0.520

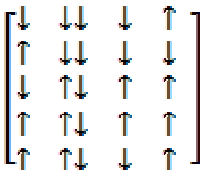
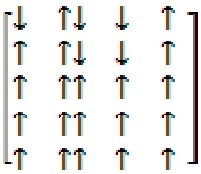

sweep9 E=-0.072,M=-0.280

sweep10 E= -0.120,M= -0.120

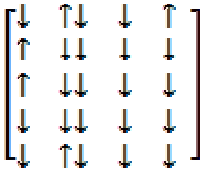
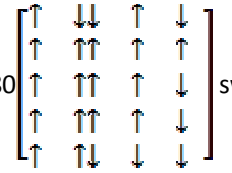
Group 6


sweep1 E= -0.000, M=-0.000

sweep2 E= -0.216, M= -0.280

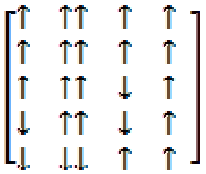
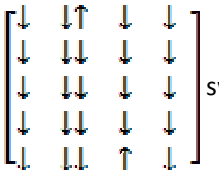

sweep3 E=-0.360, M= -0.680

sweep4 E= -0.312, M= -0.760

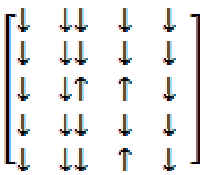
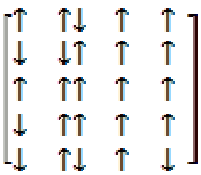

sweep5 E= -0.168, M= 0.440

sweep6 E= -0.360, M= -0.680

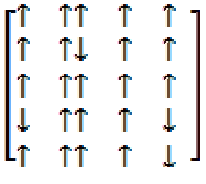
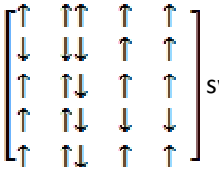

sweep7 E= -0.072, M= -0.040

sweep8 E= -0.312, M= 0.600

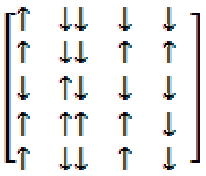
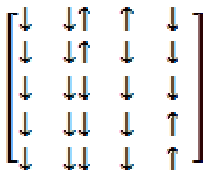

sweep9 E=-0.264, M= -0.680

sweep10 E= -0.168, M= 0.360

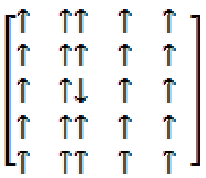
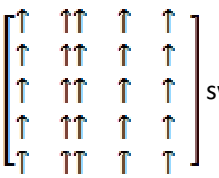
Group 7


sweep1 E= -0.216, M= 0.520

sweep2 E= -0.408, M= -0.840

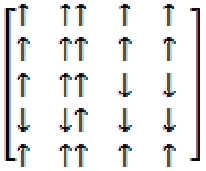
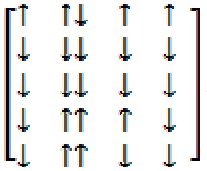

sweep3 E= -0.408, M= -0.840

sweep4 E= -0.072, M= 0.280

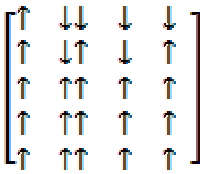
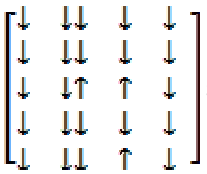

sweep5 E= -0.312, M= 0.680

sweep6 E= -0.168, M= 0.360

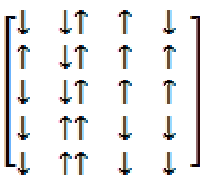
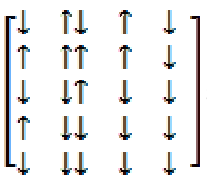

sweep7 E=-0.024, M= -0.040

sweep8 E= -0.264, M= -0.600

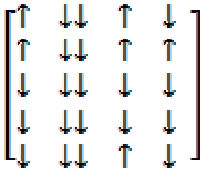
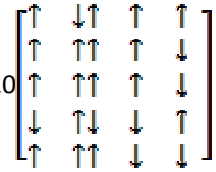

sweep9 E=-0.504, M= 0.920

sweep10 E= -0.600, M= 1.000

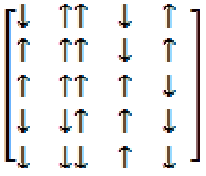
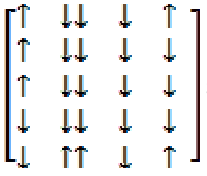
Group 8


sweep1 E= -0.312, M= 0.520

sweep2 E= -0.168, M= -0.280

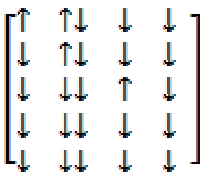
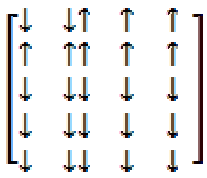

sweep3 E= -0.264, M= 0.520

sweep4 E= -0.600, M= -1.000

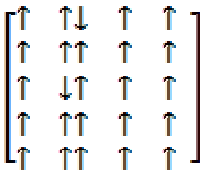
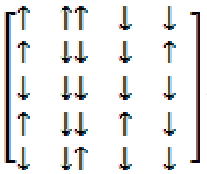

sweep5 E= -0.168, M= 0.040

sweep6 E= -0.168, M= -0.440

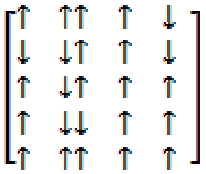
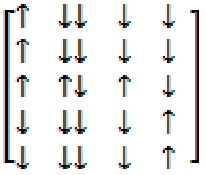

sweep7 E= -0.264, M= -0.520

sweep8 E= -0.024, M= 0.360

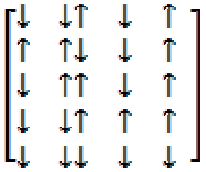
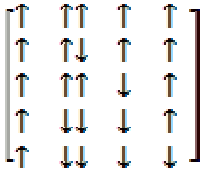

sweep9 E= -0.072, M= 0.120

sweep2 E= -0.168, M= -0.440

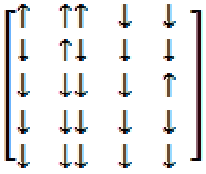
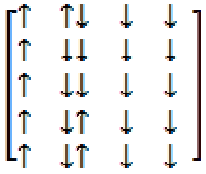
Group 9


sweep1 E=-0.312, M= -0.680

sweep2 E= -0.312, M= -0.360

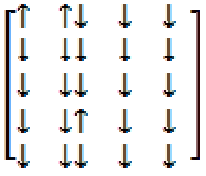
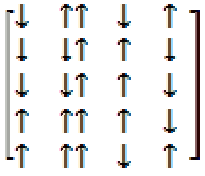

sweep3 E= -0.408, M= 0.840

sweep4 E= -0.072, M= -0.360

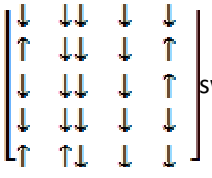
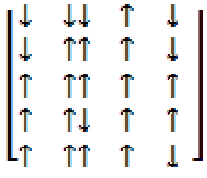

sweep5E= -0.216, M= 0.520

sweep6 E= -0.120, M= -0.440


sweep7 E= -0.024, M= -0.120

sweep8 E= -0.168, M= 0.280


sweep9E=-0.264,M=-0.600

sweep10 E= -0.168,M= -0.360

Group 10


sweep1 E= -0.360, M= -0.760

sweep2 E= -0.120, M= 0.200


sweep3 E= -0.264, M= -0.600

sweep4 E= -0.168, M= -0.440

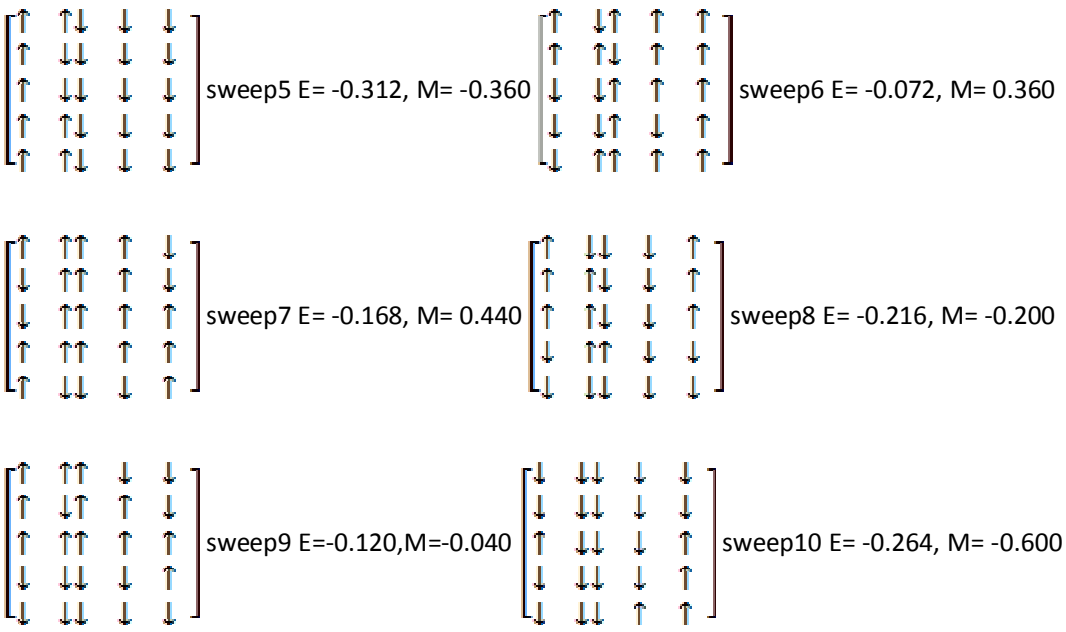


Figure 4.16 Spin –array in matrices form for 5 X 5 crystal lattice.

4.5.1 Energy E, Magnetization M, Susceptibility ^{x}, Specific heat Cv for 5 X 5 Crystal lattice

These thermodynamic functions are the data generate for 5 X 5 lattices. They are the average values per group. The averages are over ten thermalization sweeps.

Table 4.4 Tabulated values for energy, magnetization, susceptibility and specific heat

Thermalization sweep (in group)	Energy E (joules)	Magnetization M (amp/m)	Susceptibility ^{x} (dimensionless)	Specific heat C_v (joules/K/kg)
G1	-0.154	0.04	3	0.18
G2	-0.23	0.27	4.87	0.312
G3	-0.23	-0.15	6.21	0.62
G4	-0.259	0.06	6.14	0.13
G5	-0.221	-0.208	2.95	0.19
G6	-0.24	-0.16	2.21	0.19
G7	-0.29	0.144	10.88	0.77
G8	-0.22	-0.112	5.74	0.57
G9	-0.20	-0.12	5.77	0.32
G10	-0.20	-0.11	4.75	0.19

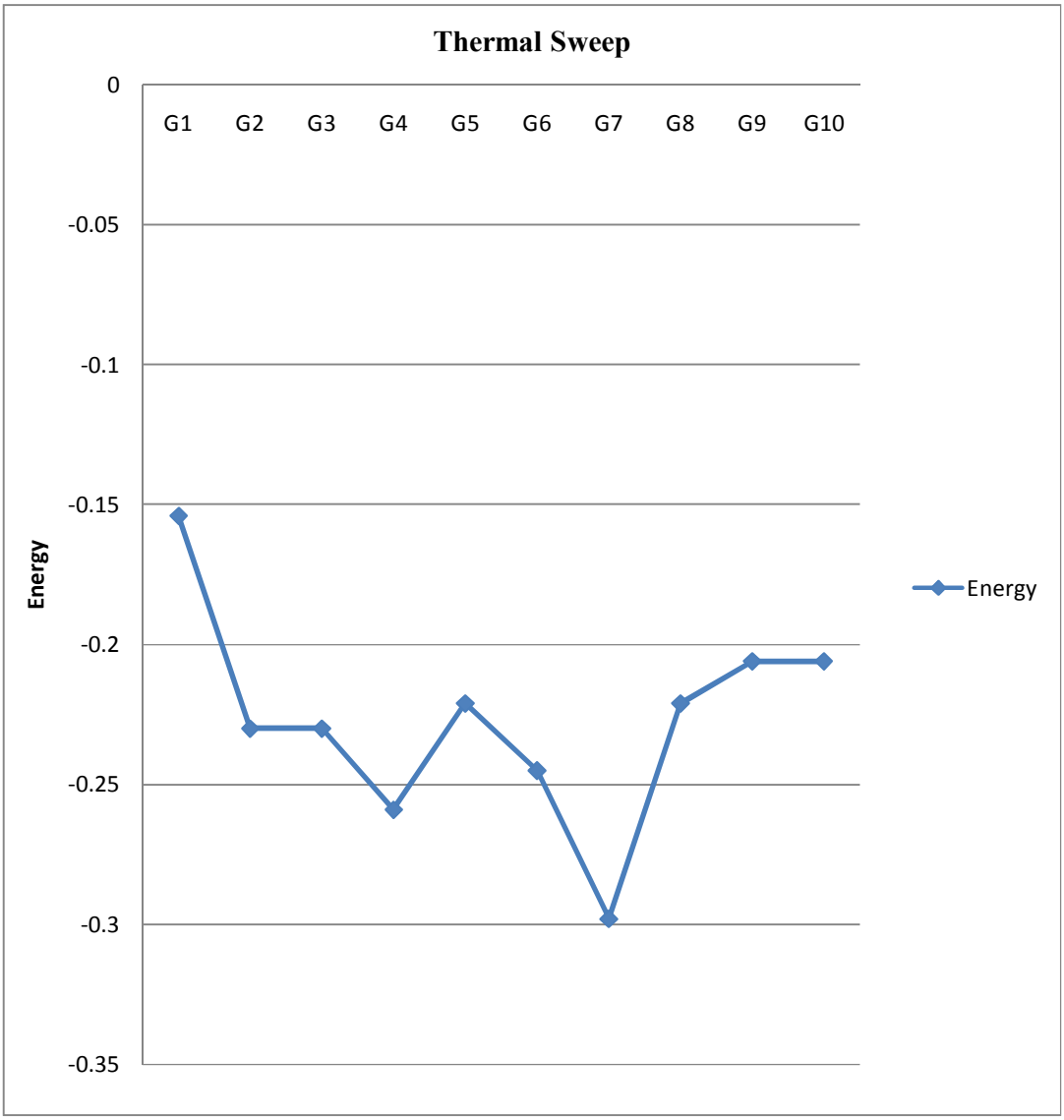


Figure 4.17 Energy as a function of thermalization sweep of 5 by 5 crystal lattice.

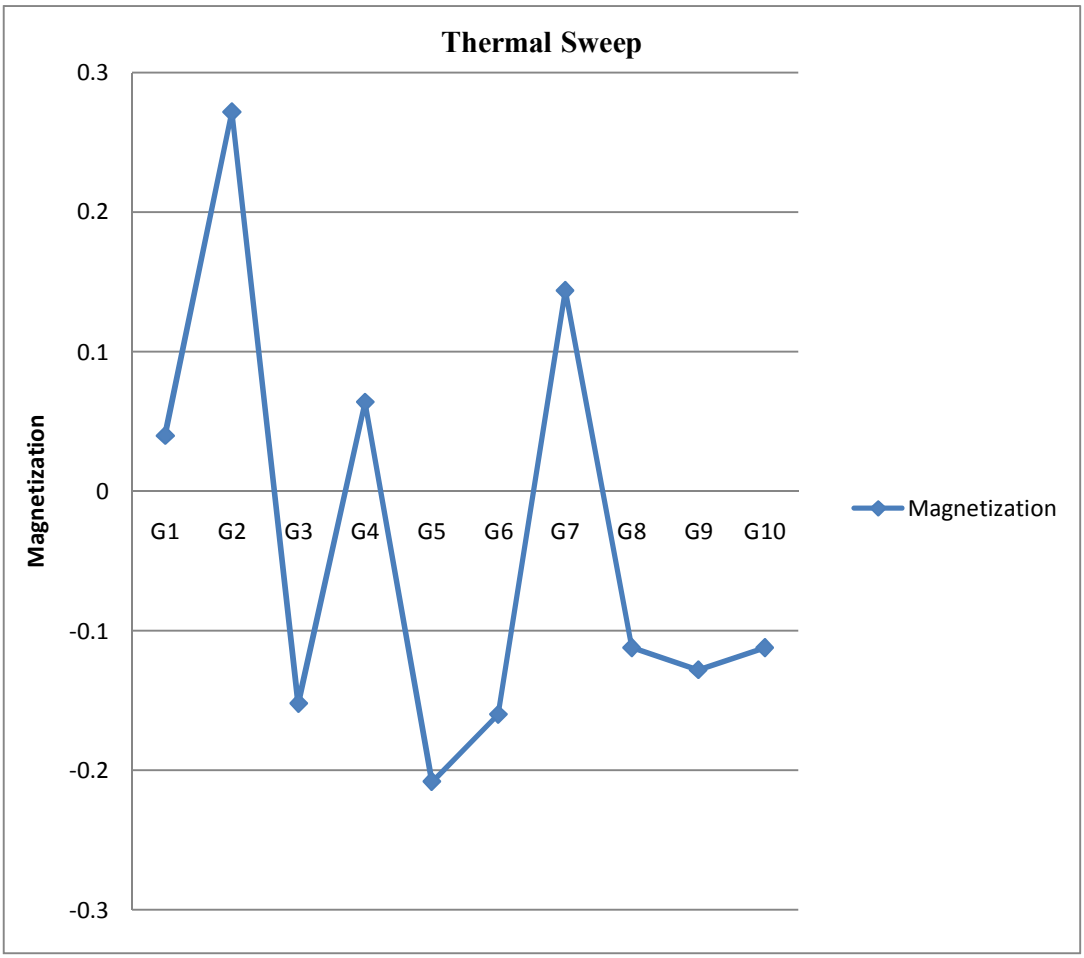


Figure 4.18 Magnetization as a function of thermalization sweep of 5 by 5 crystal lattice.

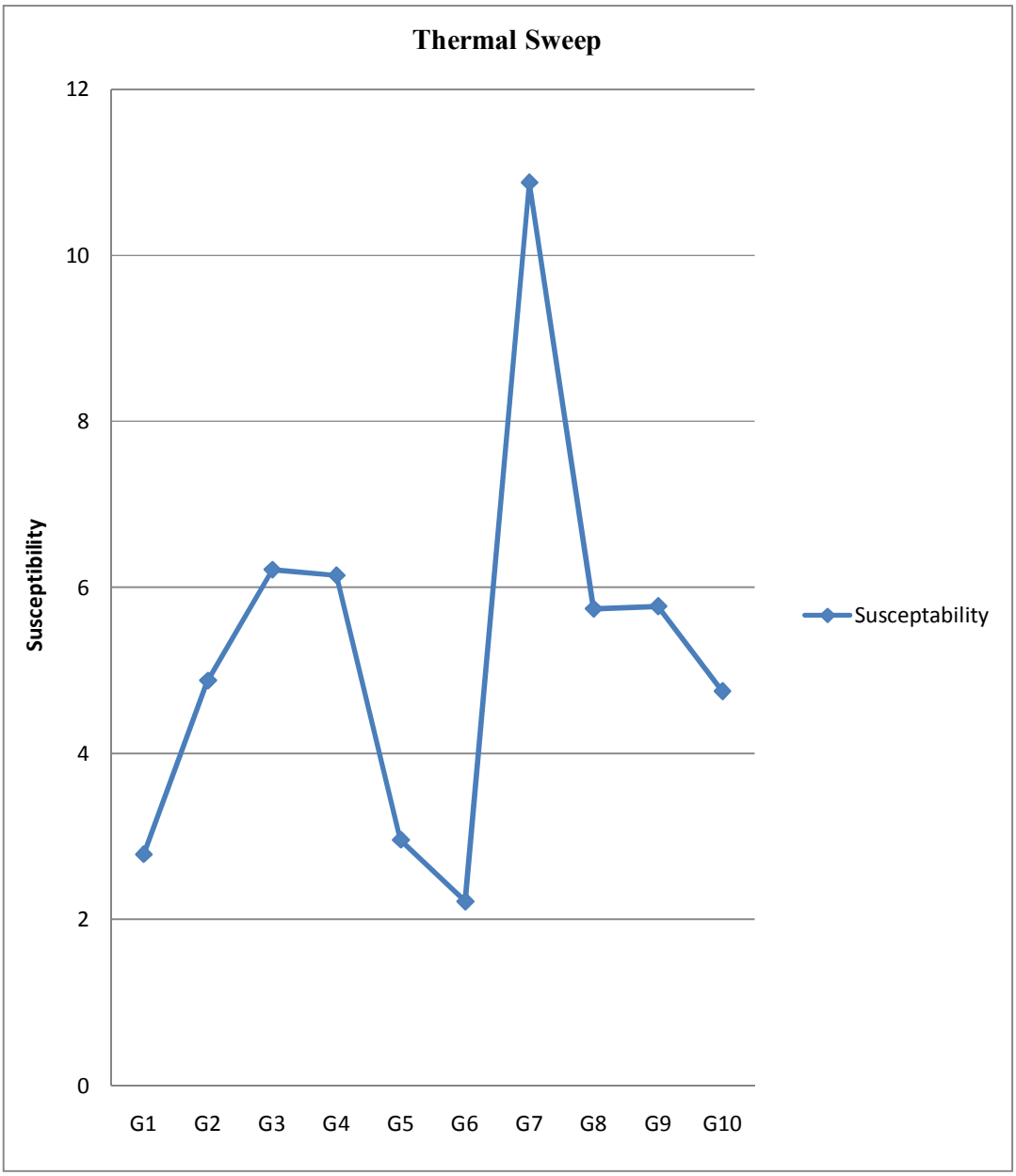


Fig. 4.19 Susceptibility as a function of thermalization sweeps of 5 by 5 crystal lattice.

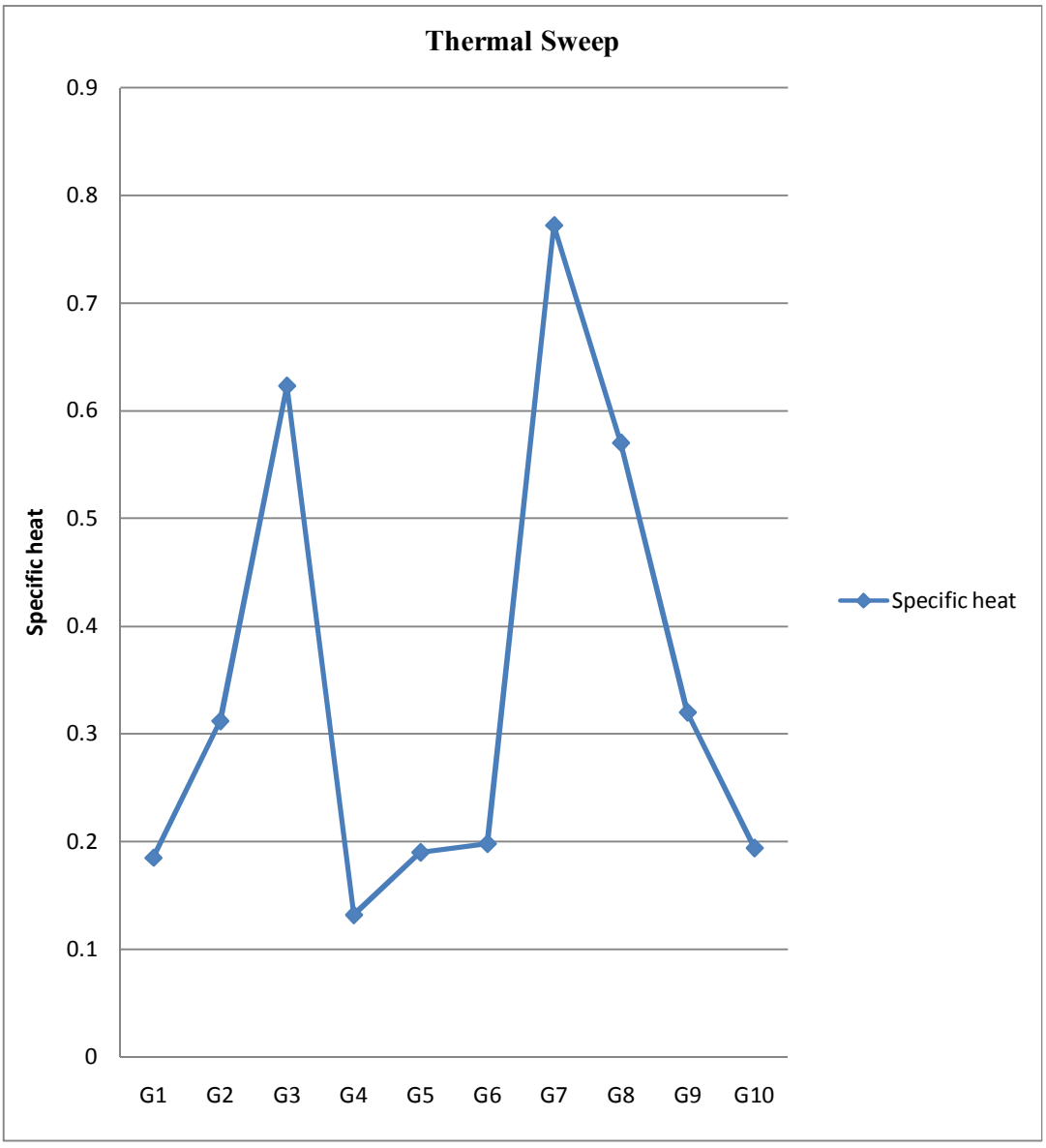


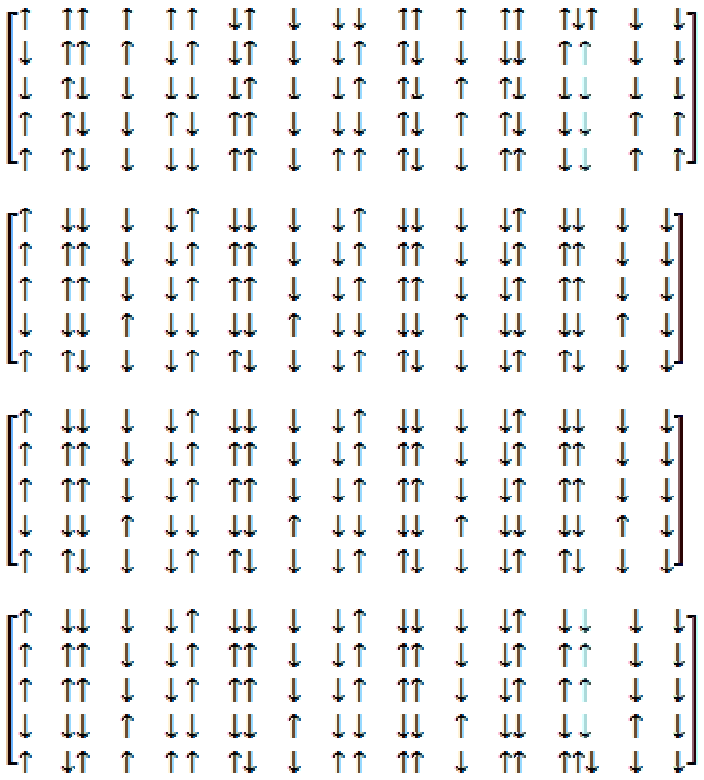
Figure 4.20 Specific heat as a function of thermalization sweep of 5 by 5 crystal lattice.

For further illustration of the above finding, the code was also simulated for a higher lattice dimension as this gives more spin alignments and a higher magnetization. Therefore few of 20 X 20 spin matrices is presented below.

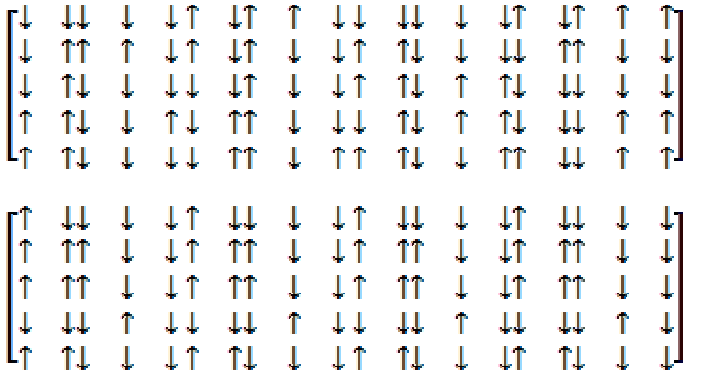
4.6 SIMULATION OF SPIN ALIGNMENT FOR 20 X 20 CRYSTAL LATTICE.

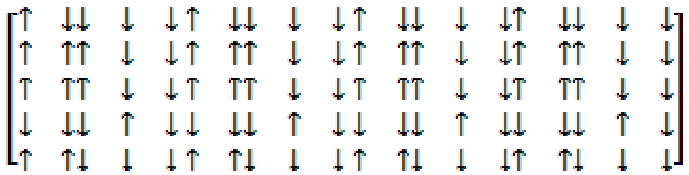
Below is the spin –array display that was obtained on running the code for 20 x 20 lattice structure under the condition of magnetic field of 0.0001 kT , interacting strength of 0.300 kT ten thermalization sweeps and ten groups respectively. The spin snapshot is presented in matrices in order to obtain accurate and precise result.

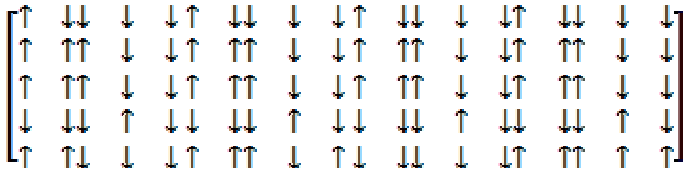
Group 1, sweep1 E=-0.201,M=-0.085



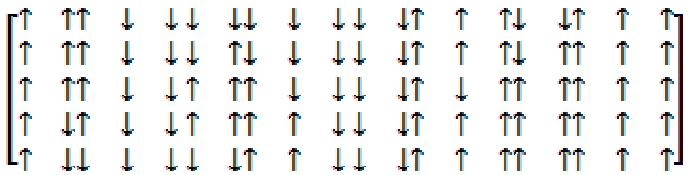
sweep2 E=-0.273,M=0.115

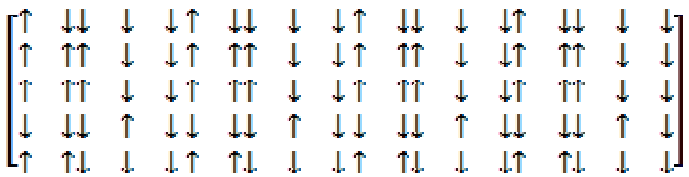


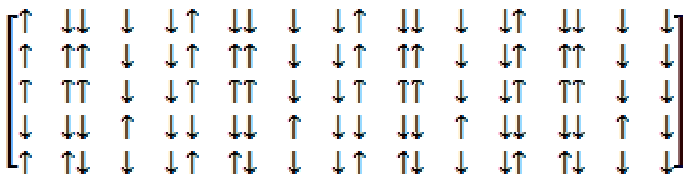


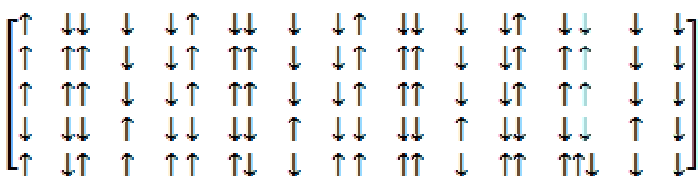


sweep3 E=-0.258,M=0.075

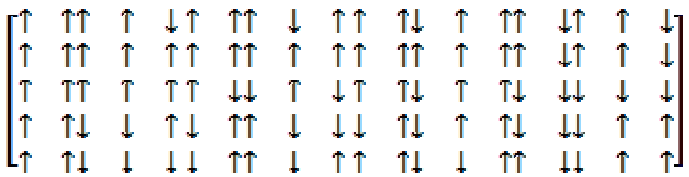


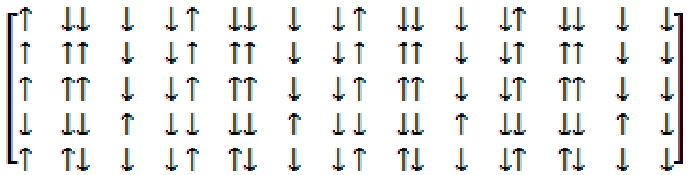


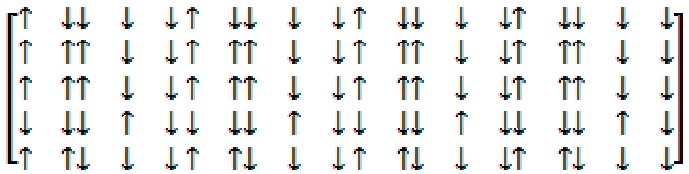


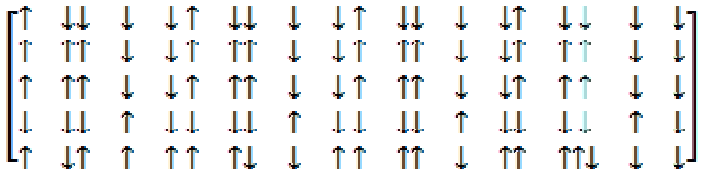


sweep4 E=-0.198,M=0.200

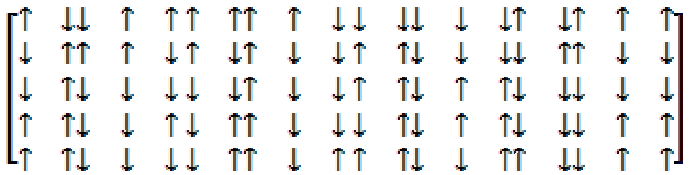


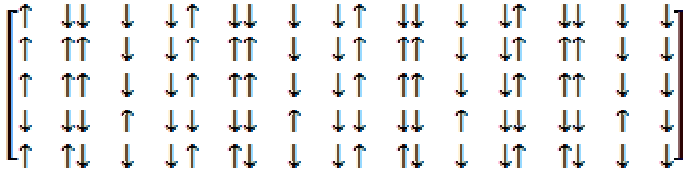


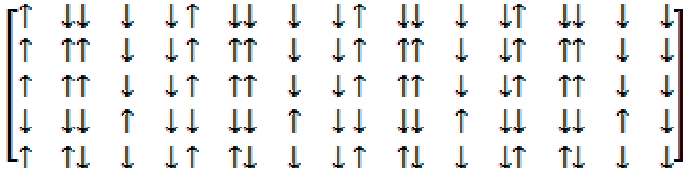




sweep5 E=- 0.204,M=0.045







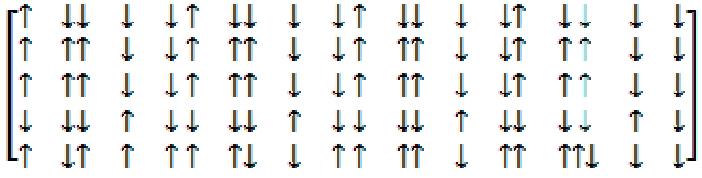


Figure 4.21 Spin –array in matrices form for 20 X 20 crystal lattice.

4.7 Energy E, Magnetization M, Susceptibility ^{x}, Specific heat Cv for 20 X 20 Crystal lattice

These thermodynamic functions are the data generate for 20 X 20 lattices. They are the average values per group. The averages are over ten thermalization sweeps.

Table 4.5 Tabulated values for energy, magnetization, susceptibility and specific heat.

Thermalization Sweep (in group)	Energy E (joules)	Magnetization M (amp/m)	Susceptibility ^{x} (dimensionless)	Specific heat C_v (joules/K/kg)
G1	-0.229	0.03	7.688	0.418
G2	-0.213	0.041	7.898	0.283
G3	-0.214	-0.158	3.392	0.131
G4	-0.2	-0.018	2.922	0.353
G5	-0.209	0.034	5.536	0.117
G6	-0.22	0.03	5.713	0.166
G7	-0.207	0.023	6.003	0.215
G8	-0.203	0.019	4.046	0.077
G9	-0.215	-0.063	3.249	0.278
G10	-0.199	-0.123	7.995	0.087

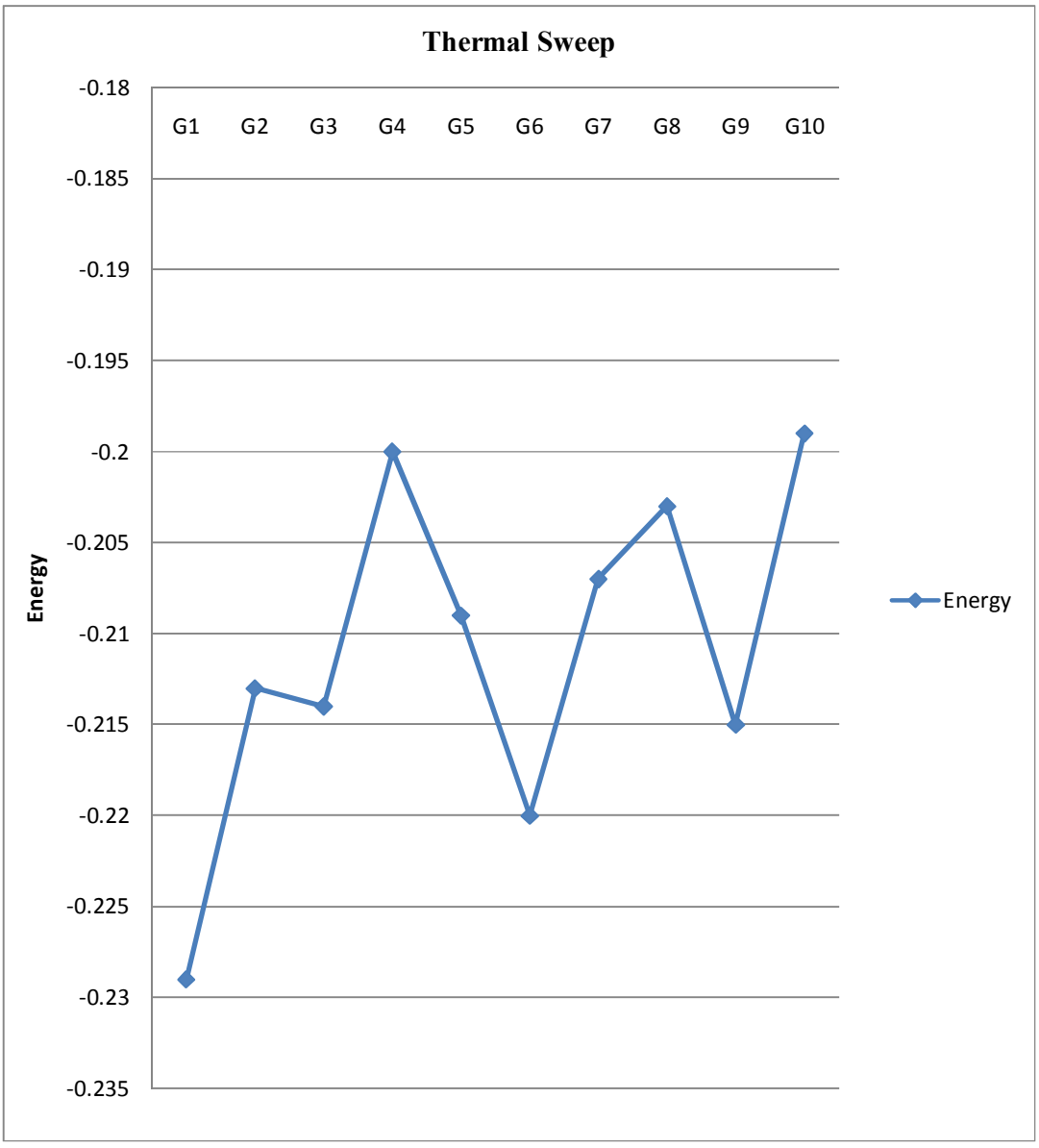


Figure 4.22 Energy as function of thermalization sweep of 20 by 20 crystal lattice.

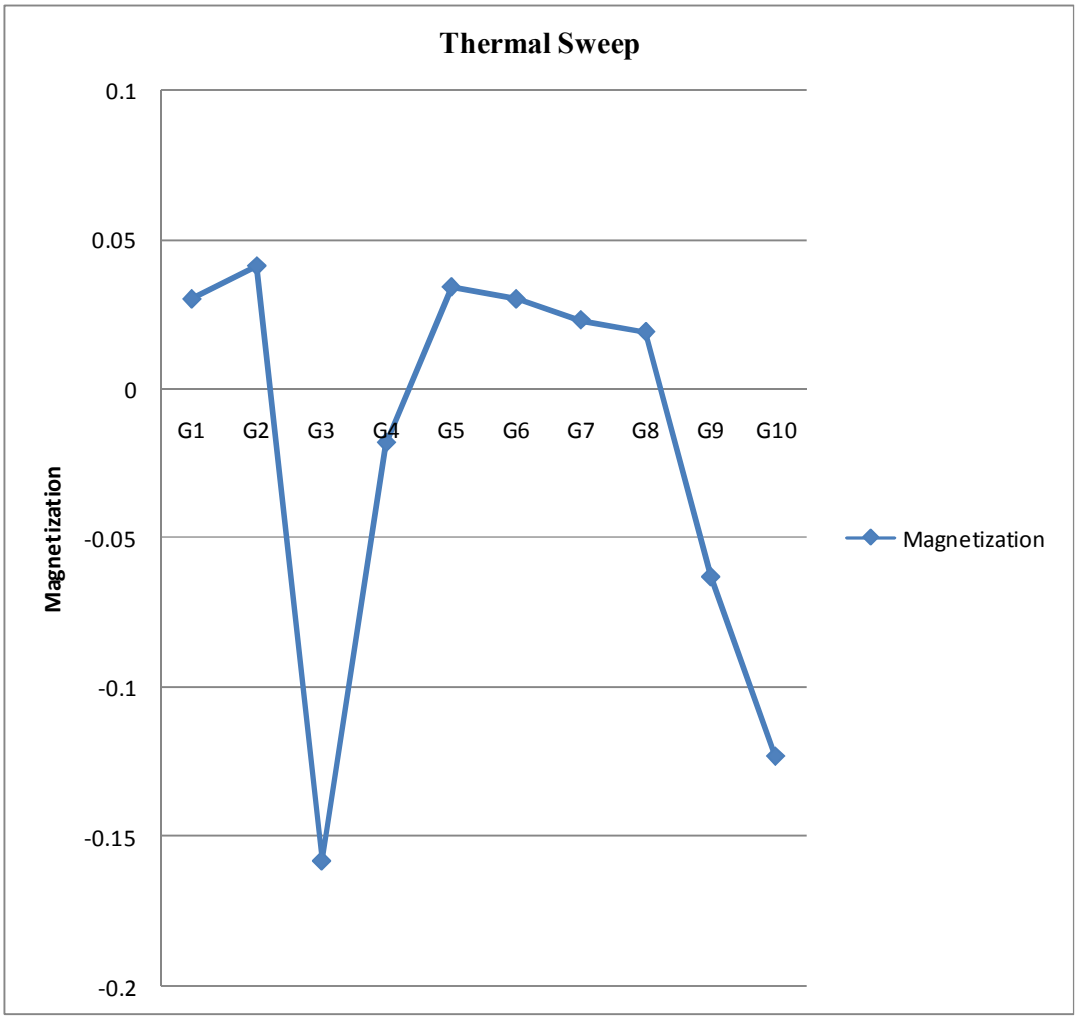


Figure 4.23 Magnetization versus thermalization sweep of 20 by 20 crystal lattice.

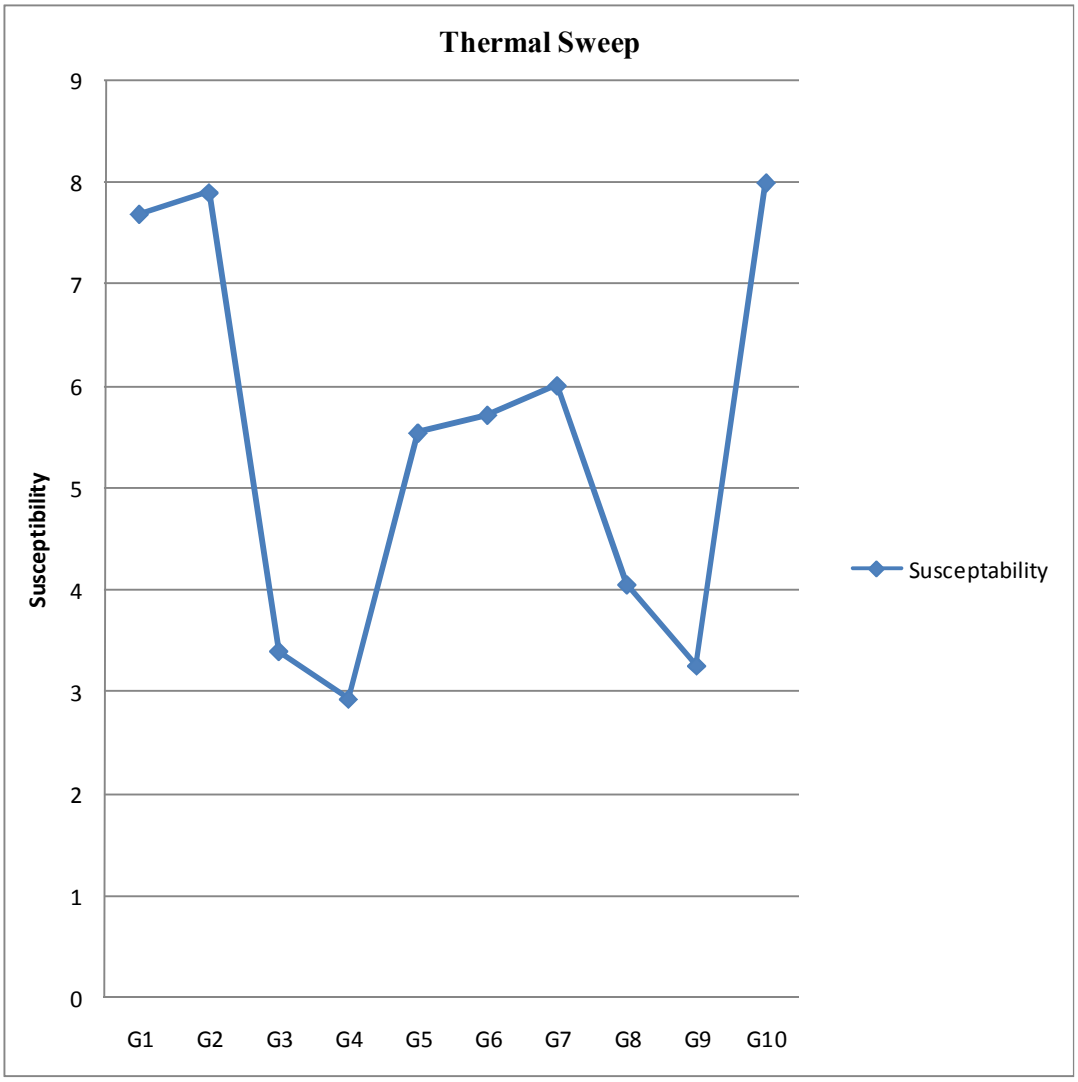


Fig. 4.24 Susceptibility versus thermalization sweep of 20 by 20 crystal lattice.

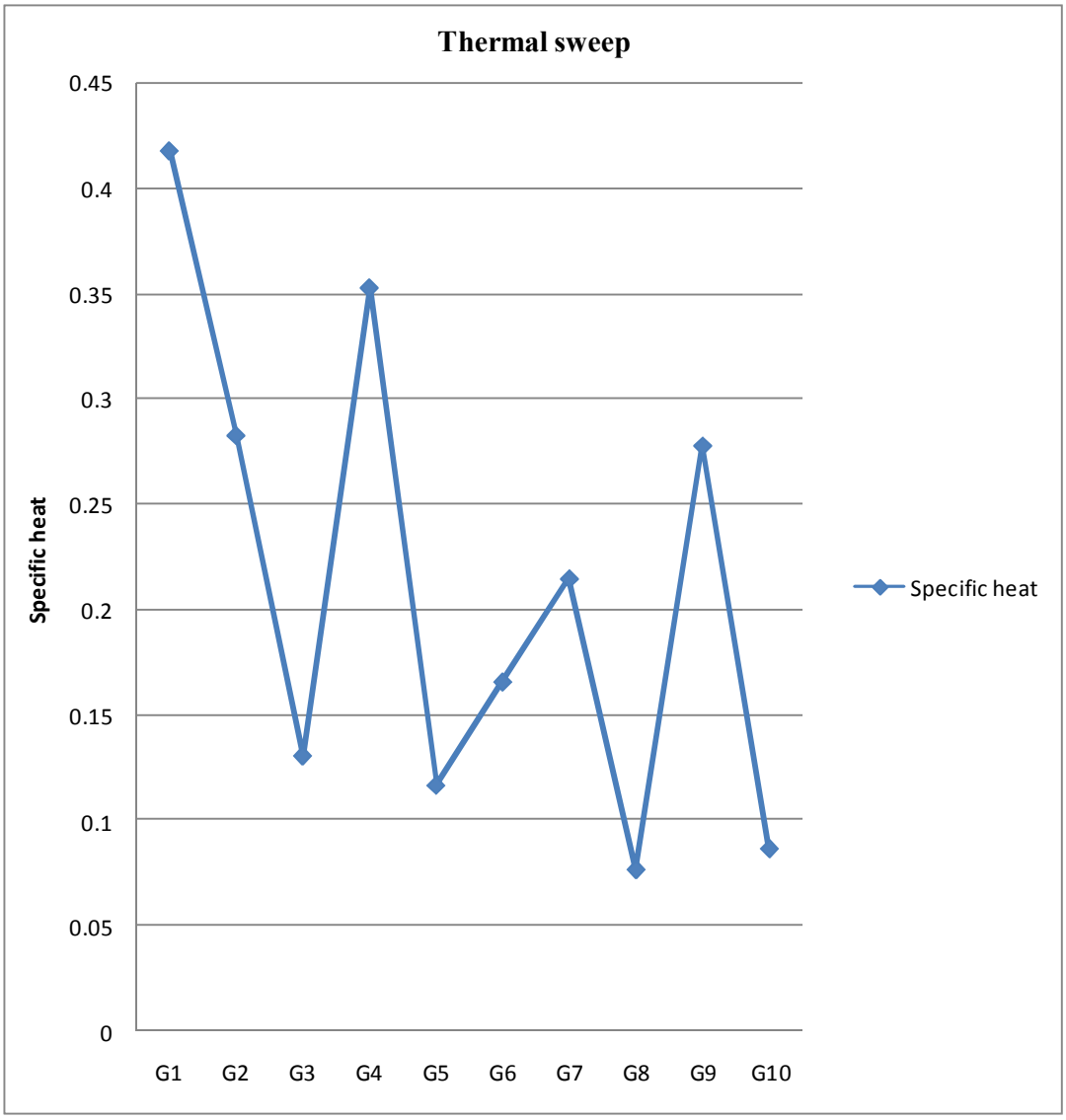


Figure 4.25 Specific heat versus thermalization sweep of 20 by 20 crystal lattice.

4.7 DISCUSSIONS

Considering the results obtained above, the arrow ↑ indicate spin alignment and more magnetization (Ferromagnetic) while the arrow ↓ indicate spin anti-alignment and less magnetization (anti-ferromagnetic) in the case of equal number of ↑and ↓, the alignment cancel out given rise to zero magnetization (non interacting spin) . From the matrices' it can be observed that "even number" thermal sweep in each group produces more spin alignment. That is in groups 2, 4, 6, 8 and 10.

It is also observed in the matrices that there is an outright anti-aligned spin with few aligned spin and a great percentage of non- alignment at all. Interestingly, the aligned spin in 2 X 2 lattices has the same value for energy and magnetization with the 3 X 3 lattice.

it is observed that for higher thermal sweep the spin remains randomly aligned after long periods of equilibration, and for low thermal sweeps, the spins end up pointing in mostly the same direction. It can be seen that spin align in an ordered form at high energy signifying spontaneous magnetization at an appropriate temperature. This spontaneous magnetization increase with increases in lattice points which further give credence to ferromagnetism being a property not just of chemical make up of a system but of its crystalline structure and microscopic organization (Bozorth, 1995).

It is also observed that aligned spins have positive values for magnetization while anti-aligned spins have a negative values for magnetization which corresponds to the fact that spins that are aligned up give a high magnetic properties in ferromagnetic system and anti-aligned spin exhibits the magnetic properties of Ferrimagnetism (Bozoth, 1995).

The graphs also shows that the system has a negative energy values, this signifies that the system is an Ising model because the Ising model has energy of a negative value as given in equation (2.13) which is justified by crystal generalization of the Heisenberg Hamiltonian in which the sum is taken over the exchange Hamiltonians for all the (*i*,*j*) pairs of atoms of the many-electron system (White,2007)

There is also an increase in the energy of the system as the number of thermalization sweep increases. This is so because as temperature increases, thermal motion, or entropy, competes with the ferromagnetic tendency for dipoles to align. If the temperature rises beyond the Curie temperature, there will be a second-order phase transition and the system will no longer maintain a spontaneous magnetization (Bozorth, 1993).

For each spin state there is a specific energy and magnetization at the end of a thermal sweep which best describes the spin state distribution.

Aside from the fact that the energy of an Ising model is negative, negative energies are also produced when you spin or rotate magnets which contain magnetic bubbles, in a magnetic field, the zero point energy (ZEP) is split, and negative energy is released which is the source of "COLD" electricity and NEGATIVE photons (Kolman, 2004)

However, the spin ↑ or ↓ distribution fluctuates with the groups, making the magnetic effect displaying an oscillating character as shown in the various graphs.

Looking at the Magnetization graph it shows that the magnetization is proportional to the excess number of spin ↑ that is aligning in the same direction. For the thermal sweep with

greater number of spin ↑, the magnetization is high. The spin tend to become randomized when thermal energy is greater than the strength of interaction. It is also observed that with increase in thermal sweep (i.e at group 9 & 10), the magnetization tends to drop because there is anti – alignments that result in zero net magnetization. Similarly there is excessive rise in magnetization at lower thermal sweep which give complete alignment of spin and magnetization keeps increasing with increase in lattice dimension also.

The susceptibility graph result indicates the degree of magnetization of the system in respond to the magnetic field applied. The Susceptibility is high compare to the small magnetic field applied. This implies that the Ising model is a complete magnetic model, because ferromagnetic system has a positive susceptibility even without external magnetic field (Bozorth, 1993).

The susceptibility increase also with more lattice dimension as it measures the degree of magnetization of the system in response to the applied field.

In this simulation, the specific heat graph indicate how the system is moving from ferromagnetic phase to paramagnetic phase. It indicates a critical temperature point where the system requires maximum thermal energy to increase its temperature. In this case the system is not required to increase in temperature above the critical Curie point, therefore the continuous decrease in specific heat. This also signifies the ferromagnetic nature of Ising model (White, 2007).

CHAPTER FIVE

CONCLUSION AND RECOMMENDATION

5.0 SUMMARY

In this work we have used atomistic Monte Carlo simulations combined with basic quantum mechanical calculations to explicitly model the spin state relaxation of a Ferromagnetic material for an experimental study on the magnetic field effects . The simulation results clearly show that highly dense and ordered spin alignment determine the degree of magnetization.

Such a result, is in agreement with the experimentally observed magnetic field effects on all the ferromagnetic metals such as Fe. Ni.Co etc, and opens the way for further investigations possibly leading to a detailed description of the complex spin distribution processes involved in the interaction between the omagnetic fields and a biomolecular system.

A generalized definition of spin-up (↑) and Spin-down (↓) for Ferromagnetism is obtained where (↑) indicates spin alignment and more magnetization effect and (↓) indicates anti- alignment and less magnetization effect.

5.1 CONCLUSIONS

The simulation procedures used in this work, establishes a more accurate and reliable method for the evaluation of energy, magnetization, susceptibility and specific heat. For a specific spin alignment, quantitative results were obtained by statistically computing them at each step of the routine (thermalization sweep).

With these result the derivative of the partition function can be easily calculated by taking the specific heat in terms of the variance of the energy.

These results have also established that before taking statistics, the system should be allowed to equilibrate for a long time (this code equilibrates for 200000 passes).

Unlike the case for the Onsager solution which is grossly approximated, the result obtained for Energy, Magnetization, and Susceptibility has an error margin of 0.006 - 0.009 which eliminates uncertainty. There was no elimination or reduction in free energy; this was possible because the collation of local energy was restricted to the nearest neighbor of lattice points so that the flipping of spin will be reduced with a probability of Boltzmann factor.

It is observed from the spin alignment that no two spin crystal structure are exactly similar, even when they exhibits same values for energy and magnetization. This validates the spin - Pauli exclusive principle(Two electrons with same spin cannot also have or occupy the same position) which directly influences the property of ferromagnetism.

The work establishes that Monte Carlo simulation has validated the various application of nuclear magnetic resonance (NMR) and magnetic resonance imaging which operates on the principle of Ferromagnetic resonance heating of Fe and Fe_3O_4 at 5.8 GHz with temperature below the curie temperature of Fe (ion) (1043K) by microwave irradiation.

5.2 RECOMMENDATIONS

The results of these work can be used in testing the range of accuracy of histogram reweighting method which determines the thermal averages at near field values. Histogram reweighting is a widely used technique of saving computer time in performing any Monte Carlo simulations at any value of applied fields which could be temperature, magnetic field, chemical potential, etc.

In carrying out further work, it is advisable that before taking statistics, the system should be allowed to equilibrate for a long time. Also the energy distribution function provides an exact benchmark for testing the evolution of statistical and systematic errors as a function of temperature.

Finally, it would be of interest for further work to be carried out in order to ascertain the occurrence of fluctuation of the spin graph.

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