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Study of Second Order Phase Transition for a Mixed Spin Ferrimagnetic System Using Landau - Expansion

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BY

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بِسْمِ اللَّهِ الرَّحْمَنِ الرَّحِيمِ

يَرْفَعِ اللَّهُ الَّذِينَ آمَنُوا مِنْكُمْ
وَالَّذِينَ أُوتُوا الْعِلْمَ دَرَجَاتٍ وَاللَّهُ بِمَا
تَعْمَلُونَ خَبِيرٌ

صدق الله العلي العظيم

Certificate

I certify that this thesis entitled " **Study of Second Order Phase Transition For a Mixed Spin Ferrimagnetic System Using Landau - Expansio**" was prepared by "**Ali Arabi Abed**" under my supervision at the department of physics, College of science, AL - Muthanna University as a part of the requirements of the Master degree of Science in physics.

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Ali Arabi.

Dedication

To my support in life

To the one who tried everything he had for me,

My Father

To the warmth of my life,

*To the one who endured every moment of pain in my life and turned it
into moments of joy*

My mother

*I owe you both what I have achieved and what I hope to reach in terms
of height*

ali arabi

ABSTRACT

In this research, magnetic phase transitions, in a molecular based magnet, have been studied using mean field method (MFM). It is worth to note, a mixed spin-(3,7/2) Blume-Capel ferrimagnetic model has been investigated. By applying Blume-Capel configuration (BCC) to a system has two sublattices with spin-3 and spin-7/2, the phase diagram of the ground-state for square and simple cubic lattices in the $(D_A/|J|, D_B/|J|)$ has been constructed. Based on Bogoliubov inequality (BI) of the free energy, it has been induced the spin compensation phenomena. Characteristic critical points, i.e., many ferrimagnetic compensation temperatures of the model have been predicted as well. New results for a cubic lattice have been given that they stimulate an experimental work in the compounds $Gd_2O_2S:Ln^{3+}$ ($Ln = Eu, Tb$). On the other hand, it has been expanded the free energy function based on Landau theory, to evaluate the second order phase transition lines experiencing the proposed system. We have established the free energy as a function of sublattices magnetizations using the canonical partition function Z . The magnetic anisotropies, i.e., crystalfield have carefully been changed so that one can examine interesting phenomena such as compensation behaviors and characteristic types for the total and sublattices magnetizations as functions of the absolute temperatures. It has been found that the proposed system has many compensation temperatures when $(-2.999 \leq D_A/|J| \leq -2.55)$ with fixed values of $D_B/|J| = -2.0$ and $D_B/|J| = -3.0$, for a simple cubic lattice ($z=6$). Besides, a series of behavior's types has been obtained for both structural lattices, which are L-, M-, type and P-, R-, S-, W- type for simple cubic and square lattices, respectively. It remains to mention that the occurrence of a compensation point is of great technological importance since at this point only a small driven field is required to change the sign of the resultant magnetization; this property is useful in reducing the area of the hysteresis loop.

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LIST OF SYMBOLS AND ABBREVIATIONS

Abbreviation	Key
A	Area (m^2)
B	Magnetic Flux Density (Tesla)
BC	Blume-Capel Model
bcc	Body-Centered Cubic
BI	Bogoliubov inequality
C	Curie Constant
c	Speed of Light in Vacuum (m/s)
D	Single-ion anisotropy or Crystal Field (J)
D_A, D_B	Single-ion Anisotropy on A and B sites, respectively (J)
e	Electron Charge (C)
fcc	Face-Centered Cubic
G	Landé g-factor
G	Free Energy (J)
H	Magnetic Field (A/m)
h	Planck Constant (J.s)
H	Hamiltonian (J)
H_0	Trial Hamiltonian (J)
h_i, h_j	Effective-Field Parameters
H_m	Molecular Field (A/m)
I	Current (A)
J	Exchange interaction (J)
k_B	Boltzmann Constant (J/k)
μ_m	Magnetic moment (A/m)
M	Total Magnetization (A/m)
m_A, m_B	Sublattice magnetizations of A and B sites, respectively (A/m)
MFA	Mean-Field Approximation

M_o	Saturation Magnetization at T=0 (A/m)
M_s	Saturation Magnetization (A/m)
N	Number of Atoms
O _i	Ordered Phase
RE	Rare Earth Metals
S	Spin Quantum Number
Sc	Simple Cubic
S _i , S _j	Spin of atoms in site <i>i</i> and <i>j</i> , respectively
T	Temperature (<i>k</i>)
T _H	Transfer Hamiltonian
T_C	Curie Temperature (<i>k</i>)
T_K	Compensation Point (<i>k</i>)
TM	Transition Metals
T_N	Neél Temperature (<i>k</i>)
W	Molecular Field Coefficient
Z	Partition function
Z	Number of Nearest Neighbors
B	Lagrange Multiplier (1/J)
M_b	Bohr Magneton (J/T)
V	Velocity (m/s)
X	Susceptibility

Chapter One

Introduction

1.1 Introduction

The history of magnetism is coincide with the history of science. The magnet's ability to attract ferrous objects by remote control [1] The magnetic material is lodestone or magnetite, which has basically the chemical constitution Fe_3O_4 or $\text{FeO} \cdot \text{Fe}_2\text{O}_3$, i. e. ferrite. It was known to the ancients that this mysterious substance had attracted other bodies of same nature [2]. All materials are magnetic, this means that every material responds to an external magnetic field in a specific manner [3].

One of the most fundamental ideas in magnetism is the concept of the magnetic field. When a field is generated in a volume of space, it means that there is a change in energy of that volume, and that an energy gradient exists, resulting in a force that can be detected by the acceleration of an electric charge moving in the field, the force on a current-carrying conductor, the torque on a magnetic dipole such as a bar magnet, or even the reorientation of spins on electrons within certain types of atoms. A magnetic dipole is represented by the torque on a compass needle, is probably the most familiar property of a magnetic field [4].

Magnetic solids are widely used in information storage devices, microwave communication systems, electric power transformers, dynamos, and high-fidelity amplifiers, to name a few.. It is by far the largest application of magnetic materials in information storage media, and the annual sales of computer disks, CDs, optical discs, tape recorders, and related items exceed those of the popular semiconductor industry. The demand for information storage media with high bit density and the emergence of new technologies such as magnetic optical devices make it imperative to expand the search for entirely new classes of magnetic materials [5].

1.2 Physical Basics Of Magnetism

The motion of an electron charge results in a magnetic field , for example , an electron loop of area A and current I produces a magnetic dipole with strength[72]:

$$\vec{M} = IA \quad (1.1)$$

Where M is magnetic moment. The current loop types of electron motion are

- 1 . The orbital motion of electrons around the atomic nucleus .
- 2 . The spin of an electron about its own axis of rotation .
- 3 . The interaction of the electron – induced magnetic moments with an externally in the macroscopic magnetic properties depend on the atomic and microstructural characteristics of a material.

An external magnetic field can be described B , or the magnetic field strength H , so :

$$B = \mu_0 H \quad (1.2)$$

This relation in a vacuum , where μ_0 is the permeability of a vacuum. A material becomes magnetized when it is placed in an external magnetic field of strength H . The extent of this magnetization can be quantified by the vector M , which represents the induced dipole moment per unit volume within the material , The total magnetic induction B is the sum of the contributions from the external magnetic field ($\mu_0 H$) and the internal response of the internal response of the material

$$B = \mu_0 H + \mu_0 M \quad (1.3)$$

Since the vector M , also known as the magnetization , is induced by the external field H it is assumed that M is proportional to H , that

$$M = \chi H \quad (1.4)$$

Where χ is the magnetic susceptibility , on

$$B = \mu_0 (1 + \chi) H = \mu H \quad (1.5)$$

1.3 Classification of Magnetic Material

Materials can be classified into five categories based on the quantity and character of the interaction between electrons in a solid and an external magnetic field. Three of these classes are paramagnetic, diamagnetic, and antiferromagnetic materials that show almost no response to external magnetic fields [6]. Ferromagnetic and ferrimagnetic materials, on the other hand, have a high interaction with external magnetic fields and can be used in a wide range of magnetic applications, including electrical transformers and information storage devices. The property that quantitatively describes the material's response to an external field is its magnetic susceptibility (χ).

Table 1.1 Periodic table shows the types of magnetic materials of all elements at room temperature [1].

PERIODIC TABLE OF THE ELEMENTS																		TM
1 1A H Hydrogen 1.008	2 2A He Helium 4.003																	18 VIIIA He Helium 4.003
3 Li Lithium 6.941	4 Be Beryllium 9.012																	10 Ne Neon 20.180
11 Na Sodium 22.990	12 Mg Magnesium 24.305																	18 Ar Argon 39.948
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.867	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.631	33 As Arsenic 74.922	34 Se Selenium 78.971	35 Br Bromine 79.904	36 Kr Krypton 84.798	
37 Rb Rubidium 85.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.95	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.905	54 Xe Xenon 131.29	
55 Cs Cesium 132.905	56 Ba Barium 137.328	57-71 Lanthanide Series	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.227	78 Pt Platinum 195.085	79 Au Gold 196.967	80 Hg Mercury 200.592	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium 209	85 At Astatine 210	86 Rn Radon 222.018	
87 Fr Francium 223.020	88 Ra Radium 226.025	89-103 Actinide Series	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [269]	109 Mt Meitnerium [268]	110 Ds Darmstadtium [269]	111 Rg Roentgenium [272]	112 Cn Copernicium [277]	113 Nh Nihonium [284]	114 Fl Flerovium [289]	115 Uup Ununpentium [288]	116 Lv Livermorium [293]	117 Uus Ununseptium [289]	118 Uuo Ununoctium [294]	
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at room temperature [1]. In the next sections, the characteristics of these materials will be discussed in thorough details.

1.3.1 Diamagnetic Material

A diamagnetic is a substance that exhibits, a negative susceptibility (negative magnetization). Despite the fact that it is composed of atoms that has zero net magnetic moment, it reacts in a certain way to the applied field, It is know the molecular currents are responsible for the magnetism in the solid materials. It has been compared the molecular currents to an electric current in a loop-shaped piece of wire, which gives rise to magnetic moment [5]. To understand the diamagnetism, an electric current has to be considered rather than molecular current. Lenz found that a current is induced in a wire loop whenever a bar magnet is moved toward (or from) this loop. Thus induced current causes a magnetic moment which is opposite to the applied magnetic field direction Fig(1.1) [9,14] . This effect is summed over all the electrons in the atom and each atom is considered to act independently of the others. All TM RE materials have diamagnetic properties, but most of these materials have other magnetic behavior, which is more dominant than diamagnetism.

1.3.2 Paramagnetic Material

Paramagnetism occurs when the atomic, ionic or molecular constituents have a non-zero magnetic moment. When an external magnetic field is applied to the specimen, the magnetic moments will be aligned with the direction of the field as shown in Figure 1.2 Hence paramagnetic materials have a positive susceptibility. The diamagnetic moments are still present, but the aligned atomic moments have a greater magnitude than the induced diamagnetic moments [14].

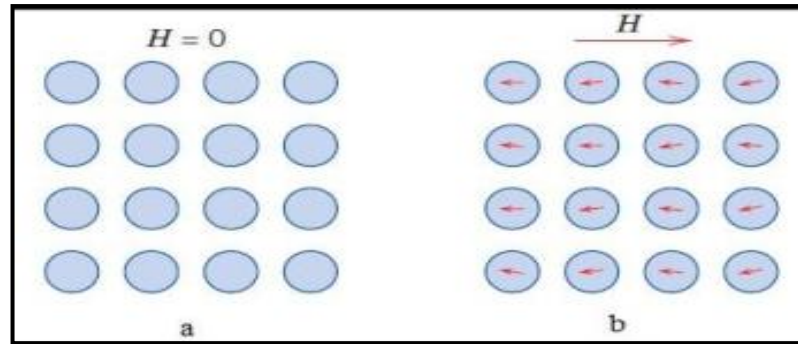


Figure 1.1: Atomic dipole for a diamagnetic material, (a) in absence of external field, and no dipoles exist. (b) In the presence of a field, dipoles induced and are aligned opposite to the field direction [5].

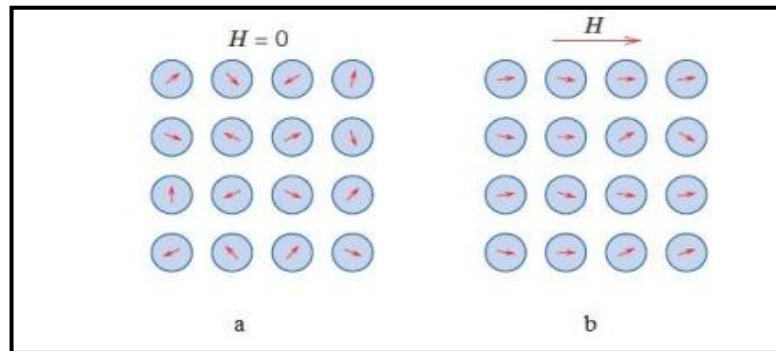


Figure 1.2: Atomic dipoles for a paramagnetic material, (a) with no applied magnetic field (b) with magnetic field [5]

The spin paramagnetism is slightly temperature dependent. It is a very weak type of magnetic behavior, which occurs in some metals, salts of the transition metals as well as rare earth metals and their salts and oxides. Curie- Weiss Law, which describes the magnetic susceptibility, in the paramagnetic region above the Curie point, can explain the temperature dependence of many paramagnetic materials that show in :- [6].

$$\chi = \frac{C}{T - T_c} \quad (1.6)$$

where, C is Curie constant depends on the material's type; T is absolute temperature, and T_c is the Curie temperature. This formula is a general of Curie's Law and it is valid only above the Curie temperature. Below T_c , the atomic magnetic moments tend to align in the same direction, which will induce a spontaneous magnetization

and the material will be in ferromagnetic phase [10]. The spontaneous magnetization below the Curie temperature arises from an internal magnetic field called the Weiss molecular field, this field is proportional to the magnetizations of small domains in the material

1.3.3 Ferromagnetism

The spontaneous magnetization attribute M , which is caused by the alignment of the magnetic moment on an atomic lattice, is a defining feature of ferromagnetism. Weiss looked at ferromagnetism through the lens of a massive internal "molecular field" proportional to magnetization [1]. It is worth to note that many paramagnetic materials, below a critical temperature, present alignment even in the absence of applied magnetic fields.

These materials, on the other hand, can be classified as ferromagnetic. When a ferromagnetic material is exposed to an external magnetic field, it becomes strongly magnetized and retains its magnetization even when the external field is removed. A very low external field of 10 A/m can also be used to produce saturation magnetization.

Many materials, such as transition or irons group elements (e.g. Fe, Ni, Co) and rare earth group elements (e.g. Gd or Dy), exhibit ferromagnetic properties, as seen in Table 1.1 besides many other compounds and alloys [5,10,13] . When a ferromagnetic material is heated to its critical temperature (Curie point), the magnetic dipoles gain thermal energy, increasing their thermal agitation and, as a result, rotating in a random manner. This disorder of the magnetic moments is the paramagnetic phase. Different ferromagnetic materials have different values of Curie temperature [5].

1.3.4 Antiferromagnetic Material

Antiferromagnetism is a mysterious magnetic order in which a crystal lattice is partitioned into two or more atomic sublattices, which order so that their net magnetization is zero. [6]. When studying the antiferromagnetic behavior of magnetic moments, it was discovered that neighboring spins are oriented antiparallel to each other, causing their magnetic spins to cancel out, resulting in a very modest positive susceptibility of 10^{-5} to 10^{-2} . Neel is primarily responsible for the development of antiferromagnetism theory, in which he applied molecular field theory to the problem as fig1.3 [9,13]. ,

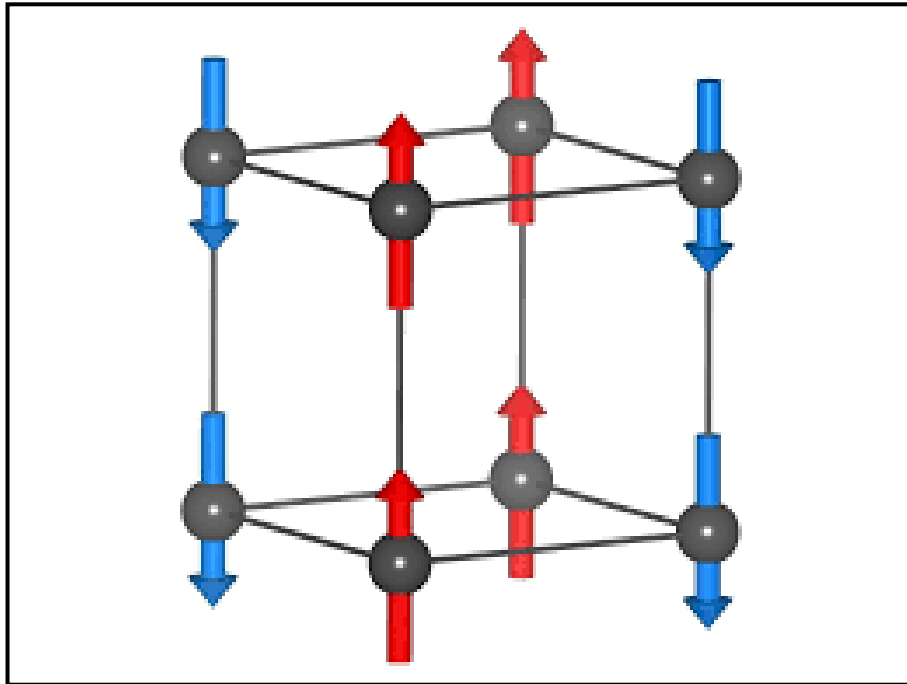


Figure 1.3: Schematic representation of antiparallel alignment of magnetic of antiferromagnetism [5]

Antiferromagnetic susceptibility varies with temperature as shown in Figure 1.4 As the temperature decreases, χ increases that it goes through a maximum point which is a critical temperature called Neel temperature T_N and usually it is less than room temperature, which indicates that with the appropriate measurement, a given paramagnetic material could be antiferromagnetic at low temperatures [9,13]. Weiss's

theory explains the temperature dependence of the susceptibility by understanding the magnetic ordering.

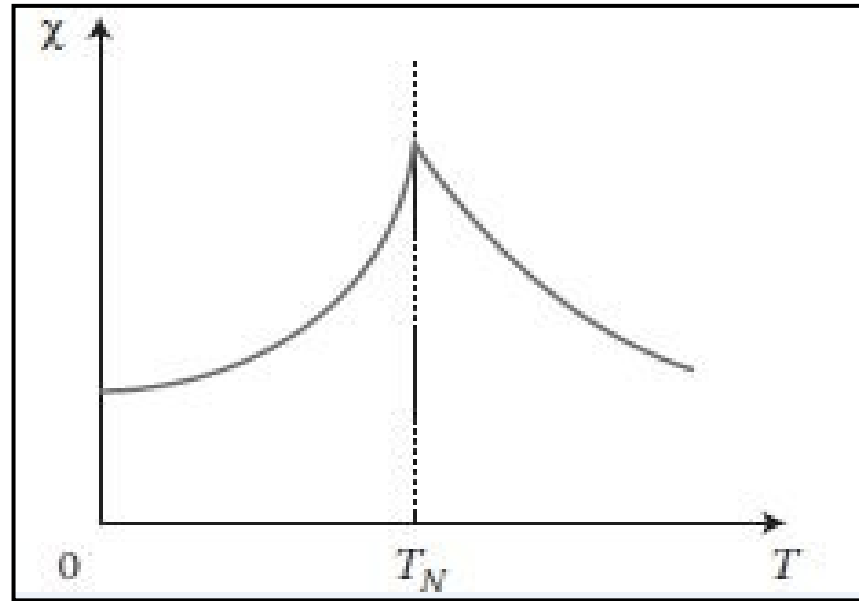


Figure1.4 Antiferromagnetic susceptibility varies with temperature[6].

Before the publication of Neel's classic paper, it was known experimentally that the susceptibility of antiferromagnets depends on the temperature, as shown in Figure 1.5 [6]. For temperatures greater than a critical one, the susceptibility follows the paramagnetic Weiss's law but with a negative value of θ as shown in Eq(1.7). Therefore, ferromagnets and antiferromagnets are akin at high temperatures , that :

$$\chi = \frac{C}{T - (-\theta)} \quad 1.7$$

Below the critical temperature i.e; Neel temperature, the system becomes ordered. Therefore, the susceptibility decreases with decreasing temperature because of the tendency for the antiparallel alignment increases. Table1.2 shows Curie's temperature for different ferromagnetic materials [8].

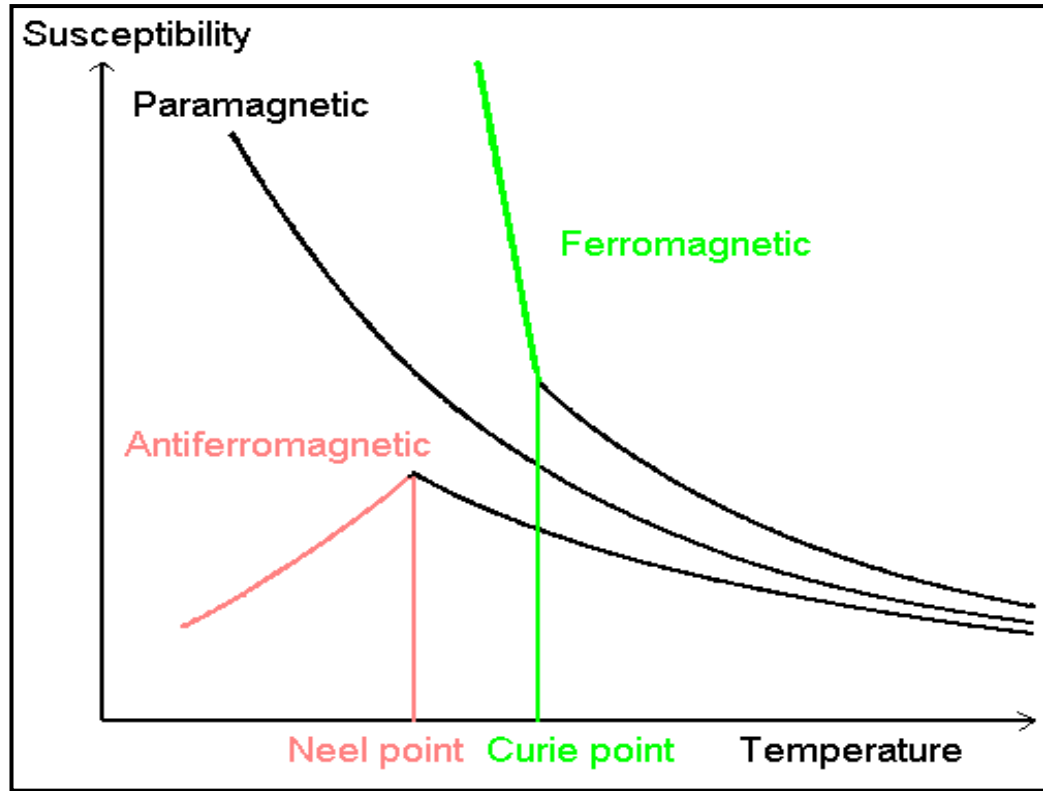


Fig 1.5: Temperature dependence of susceptibility for antiferromagnetic materials [13]

Table 1.2: Curie's Temperature for different ferromagnetic materials [8].

Material	Curie temperature
<i>Iron</i>	<i>770°C</i>
<i>Nickel</i>	<i>380°C</i>
<i>Cobalt</i>	<i>1130°C</i>
<i>Gadolinium</i>	<i>20°C</i>
<i>Terfenol</i>	<i>380-430°C</i>
<i>Nd₂Fe₁₄B</i>	<i>312°C</i>
<i>Alinco</i>	<i>850°C</i>
<i>SmCO₅</i>	<i>720°C</i>
<i>Hard ferrites</i>	<i>400-700°C</i>
<i>Barium ferrite</i>	<i>450°C</i>

1.3.5 Ferrimagnetic Materials

The magnetic moments of one kind of ion at one lattice site aligned antiparallel to those of ions in another lattice site in a ferrimagnet. Because the magnetic moments are not at the same magnitude, they only partially cancel each other, which means that the material has a net magnetization. Ferrimagnetism has several similarities to ferromagnetism in that the mutual alignments between magnetic dipoles produce a net magnetic moment even in the absence of an applied field [7]. The difference between magnetic dipoles alignment of the ferromagnetism, antiferromagnetism, and ferrimagnetism is demonstrated see Figure 1.6).

Ferromagnetic 	Below T_C , spins are aligned parallel in magnetic domains
Antiferromagnetic 	Below T_N , spins are aligned antiparallel in magnetic domains
Ferrimagnetic 	Below T_C , spins are aligned antiparallel but do not cancel
Paramagnetic 	Spins are randomly oriented (any of the others above T_C or T_N)

Figure 1.6: Magnetic moments spin arrangements for a ferromagnet, an antiferromagnet, a ferrimagnet and paramagnetic [14].

The presence of negative exchange interaction among the magnetic ions (atoms) associated with the distinct sublattices is a crucial requirement for the formation of ferrimagnetic arrangement. Ferrimagnetism can be found in both crystalline and amorphous magnetic materials, such as alloys, in the temperature range of 0 to Neel point T_N [17]. A large number of ferrimagnets are known; the main class is the ferrites. There are three types of ferrites: cubic (spinal), hexagonal

and garnet table 1.3. Cubic ferrites have a general formula $MO \cdot Fe_2O_3$, where M is a divalent metal like Mn, Ni, Fe, etc. Hexagonal ferrites have the formula $MO \cdot 6Fe_2O_3$ such as barium ferrite, $BaO \cdot 6Fe_2O_3$. Garnets are oxides with rare earth metals having general formula $5Fe_2O_3 \cdot 3M_2O_3$. Here M stands for a trivalent element such as gadolinium, yttrium, terbium etc.

Tabel 1.3 There are three types of ferrites: cubic (spinal), hexagonal and garnet

Ferrite Type	Structure	General formula	Example
Spinel	Cubic	Me_2O_4	M = Ni, MN, Co, Cu, Mg, Zn e.g., $Cu Fe_2O_4$
Garnet	Cubic	$3R_2O_3 \cdot 5 Fe_2O_3$	R = Dee, God, Ho, PR, By Y, Ms., Au, Err, Lu e.g., $3Y_2O_3 \cdot 5Fe_2O_3$
Magnetoplumbite	Hexagonal	$Me_{12}O_{19}$	M = Ba, Sir, Pub, CA e.g., $BaO \cdot 6Fe_2O_3$
Orthoferrites	Perovskite	$RFeO_3$	Dee, Err, Y, By R is rare earth

In table 1.4 shows some common ferrimagnetic materials with their critical and compensation temperatures [12,14]. It is already mentioned that ferrimagnets are similar to ferromagnets, which have a non-zero net magnetization below Curie's point (critical temperature) and does not show any magnetic ordering of the spins above this point and then it reveals a paramagnetic properties. Nevertheless sometimes, there is a temperature below the critical temperature, at which the sublattice magnetizations are equal in magnitude having antiparallel arrangements produces zero net magnetization

Table 1.4: Some common ferrimagnets with their critical and compensation temperatures z

Materials	Sublattices	T_c (K)	T_{comp} (K)
Fe_3O_4	$8a;16d$	856	
$\text{YFe}_5\text{O}_{12}$	$16a;24d$	560	
$\text{BaFe}_{12}\text{O}_{19}$	$2a,2b,4f1,4f2,12k$	740	
TbFe_2	$8a,16d$	698	
GdCo_5	$1a,2c,3g$	1014	287

. This temperature is known as compensation point. Figure 1.7 illustrates the difference in magnetization and susceptibility between ferromagnets and ferrimagnet with respect to temperature [12].

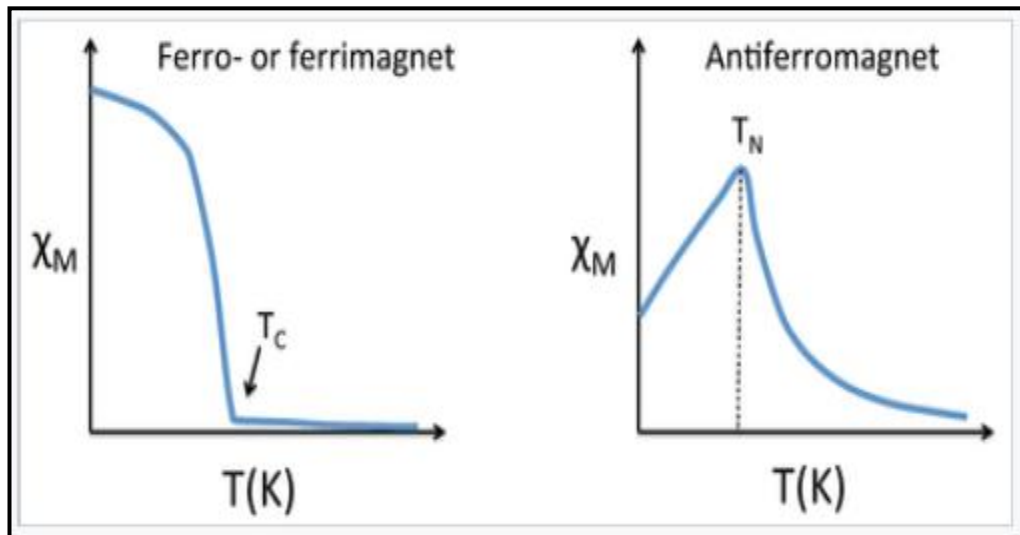


Figure 1.7: Comparison of magnetization and inverse susceptibility in typical ferromagnetic and ferrimagnetic materials [13].

1.4 Effects Temperature on Magnetization

One can investigate the temperature dependence of the spontaneous magnetization as well. This is done by using the graphical solution, assuming that[14]

$$H = H_w, \text{ then}$$

$$\alpha = \frac{mH_w}{k_B T} = \frac{m\gamma M}{k_B T} \quad (1.8)$$

So

$$M = \left(\frac{k_B T}{m\gamma} \right)_{\alpha} \quad (1.9)$$

The magnetization is a linear function of α with slope proportional to the temperature. So as the temperature increases, the slope of the dashed line increases, and it intersects the Langevin function at a point corresponding to a smaller spontaneous magnetization, M_{spont} . Eventually, when the gradient of the dashed line approaches the tangent to the Langevin function at the $\alpha = 0$ limit, the spontaneous magnetization is zero. This is shown by the straight dotted line in Figure 1.9. The temperature at this point is the Curie temperature, and at any higher temperature the *only* solution is at the origin, meaning that the spontaneous magnetization vanishes. The magnetization decreases smoothly to become zero at $T = T_C$, indicating (see Figure 1.8 that the ferromagnetic to paramagnetic transition is a second-order phase transition [14].

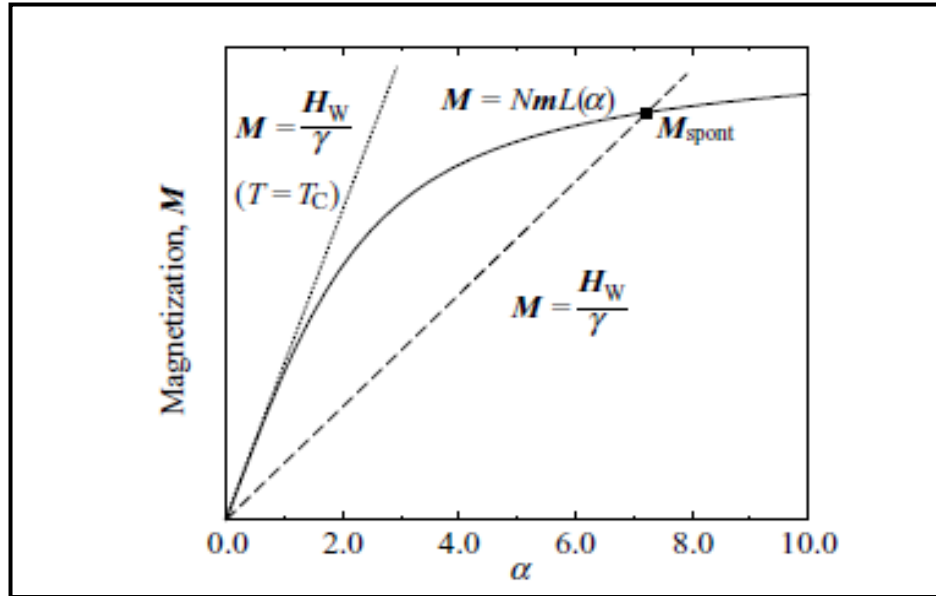


Figure 1.8 The spontaneous magnetization is zero [14]

The Curie temperature can be determined by equating, at the origin, the slope of the magnetization described by the Langevin function (which is $1/3 \times Nm$), with the slope of the straight line representing magnetization by the molecular field:

$$\frac{k_B T}{m\gamma} = \frac{1}{3} \times N_m \quad (1.10)$$

$$T_C = \frac{\gamma N m^2}{3k_B} \quad (1.11)$$

A large molecular field constant leads to a high Curie temperature. This is what we would expect intuitively – magnetic moments which interact strongly with each other should require a larger thermal energy to disrupt their magnetic ordering and induce a phase transition to a paramagnetic phase. Conversely, if the Curie temperature is known, then the Weiss molecular field can be extracted:

$$\gamma = \frac{3k_B T_C}{N m^2} \quad (1.12)$$

Greater accuracy can be obtained by replacing the Langevin function with the quantum mechanical Brillouin function, with an appropriate choice of J . Using the quantum mechanical expressions, the molecular field constant is given by[14].

1.5 literature review

Unlike ferromagnets and antiferromagnets, ferrimagnetism has been one of the most intensely investigated subjects in statistical mechanics and condensed matter physics in recent decades due to its wide range of applications in technologically relevant materials.. Ferrimagnets have a high possibility of having a compensation temperature under certain situations. Absolute magnetization vanishes below the critical temperature. In a hysteresis loop, the inclusion of a compensation temperature is critical because it allows a modest directed field to modify the sign of the total magnetization.

In 1999 G. M. Buendía and R. Cardona, introduced The magnetic properties of a mixed Ising ferrimagnetic model on a square lattice, in which the two interpenetrating square sublattices have spins that can take two values, $s=\pm 1/2$, alternated with spins that can take four values, $S=\pm 3/2, \pm 1/2$ [15].

In 2000 N. Benayad, A. Fathi, R. Zerhouni, studied the diluted mixed-spin transverse Ising system consisting of spin-1/2 and spin-1 with crystal field interactions is studied by the use of an effective field method within the framework of a single-site cluster theory. The state equations are derived using a probability distribution method based on the use of Van der Waerden identities. The complete phase diagrams are investigated in the case of the honeycomb lattice [16].

In 2000 A. Dakhama and N. Benayad suggested an exactly solvable mixed spin-1/2 and any arbitrary spin- $1/2$ Ising ferrimagnetic model. Although the system with only an antiferromagnetic interactions J between pairs of nearest-neighbor spins and crystal fields does not undergo a compensation point. However the system with additional interactions between spins does. At last, they have discussed the origin of compensation phenomenon[17].

In the same year Y. Nakamura et al. studied the magnetic characteristics of a diluted mixed spin-2 and spin-5/2 ferrimagnetic Ising model by using the effective-field theory taking the correlation between spins into account. The effects of transverse fields and concentration of magnetic atoms on the magnetic properties have been investigated numerically[18].

O.F. Abubrig et al. in 2001 have studied the mixed spin-1 and spin-3/2 Ising ferromagnetic system with different anisotropies by using MFA based on Bogoliubov inequality for Gibbs free energy. The main phase diagrams have been

obtained in the temperature-anisotropy plane. Besides, the presence and dependence of the compensation points on the crystal field have been investigated[19].

In 2000 Yasuki Nakamura studied the existence of compensation temperature of a mixed spin-2 and spin-5/2 Ising ferrimagnetic system on a layer honeycomb lattice the effect of a single-ion anisotropy and interlayer interaction on the compensation phenomenon in order to clarify the characteristic feature observed in a series of molecular-based magnets $AF^{II}FE^{III}(C_2O_4)_3[A=N(n-C_nH_{2N+1})_4, n=3-5]$. They carried out Monte Carlo simulations and found that an interlayer interaction plays one of the roles for the existence of a compensation point when there are clear differences between the ideal Ising systems and real materials [20].

In 2000, W. Wolf has shown certain magnetic materials behave similarly to corresponding Ising models. The author extensively studied materials include $Dy(C_2H_5SO_4)_3 \cdot 9H_2O$ (DyES), $Dy_3Al_5O_{12}$ (DyAlG), $DyPO_4$, $Dy_2Ti_2O_7$, $LiTbF_4$, K_2CoF_4 , and Rb_2CoF_4 . The results have been found a good agreement with the experimental ones [21].

In 2000, David N. Hendrickson et al., determined the reaction of $[Mn_3O_2(X\text{-benzoato})_6L_3]$ (X = Cl, Br; L = pyridine) with 2,2'-bipyridine in CH_2Cl_2 leads to the high-yield formation of two new mixed-valence manganese complexes of formula $[Mn_4O_2(X\text{-benzoato})_7(bpy)_2]$ (X = 2-Cl, 2-Br) and the crystal structure of the 2-Cl complex: Ground-State Spin Variability in the $[Mn_4O_2]_{7+}$ complexes [22].

In 2002 J.V. Alvarez et al. obtained a microscopic model for a class of mixed-spin quantum antiferromagnets that describes the magnetic behavior of the mixed-spin ($s=1$ and $s=1/2$) quantum systems R_2BaNiO_5 (R = magnetic rare earth). An evaluation of the properties of this model by quantum Monte Carlo simulations

shows remarkable good agreement with the experimental data, and provides insight into the physics of mixed – spin quantum magnets [23].

In 2002 M.Dantziger et al , calculated In –plane dipole coupling anisotropy of a square ferromagnetic Heisenberg monolayer this anisotropy increasing temperature , reaching its maximum value close to the Curie temperature of the system . The reason for the dipol-copling induced anisotropy is the disturbance of the square spin lattice due to thermal fluctuations (" order-by-disorder"effect). The results are obtained from a Heisenberg Hamiltonian by application of a mean field approach for a spin cluster [24].

In 2003, Wei Jiang et al. introduced an effective field theory for a mixed spin-1 and spin- 3/2 with different anisotropies in a transverse field of a honeycomb lattice. The calculation of the temperature dependence of total magnetization has been examined to determine the phase diagram of the transition temperatures. Some interesting phenomena occurred, such as the presence of two tricritical points and the existence of the two compensation points [25].

In 2004 W.Figueiredo et al, introduced a layer mixed – spin model, with spins $s_i=1/2$ and $s_j=1$, distributed on the sites of a hexagonal lattice . For this spin arrangement , any spin at one lattice site has two nearest – neighbour spins of the same type, and four of the other type . They assumed that the exchange interaction between spins s_i and s_j antiferromagnetic, with the value J_1J_2 is the exchange interaction between two nearest neighbor spins [26].

In 2004 Guang- Shan Tian and Hai-Qing, suggested the quantum phase transition and ferrimagnetic long- rang order in the mixed – spin Heisenberg model with single –ion anisotropy on a bipartite lattice ,when the single – ion anisotropy

energy D is positive, the model has a unique ground state with the total spin $-z$ component [27].

In 2005 W.T.Lu et al soluble kagome lattice Ising model in a magnetic field is solved exactly under the presence of a nonzero external magnetic field. The model generalizes the superexchange model introduced by Fisher in 1960 and is analyzed of its thermodynamic and magnetic properties [28].

In 2006 J Oitmaa and I.G.Enting, They used both high- and low-temperature series to investigate the phase diagram of a ferrimagnetic mixed-spin $(1/2,1)$ Ising model on the square lattice, including an on-site anisotropy term on the $S=1$ sites [29].

A. Benyoussef et al. (2007) examined the magnetic properties of a decorated ferrimagnetic mixed spin- $1/2$ and spin-1 Ising model consisting of two sublattices A and B by the use of mean field approach. For the decorated ferrimagnetic square lattice, the transition and compensation temperatures have been investigated [30].

In 2008 A. E. Berkowitz, et al, report the magnetic and microstructural properties of antiferromagnetic MnO nanoparticles with shells of ferrimagnetic Mn₃O₄, which is opposite the usual arrangement of antiferromagnetically coated ferromagnetic nanoparticles [31].

In 2009 Rachidi A. Yessoufo et al, used exact recursion relations to study the magnetic properties of the half-integer mixed spin- $5/2$ and spin- $3/2$ Blume-Capel Ising ferromagnetic system on the two-fold Cayley tree that consists of two sublattices A and B. Two positive crystal-field interactions Δ_1 and Δ_2 are considered for the sublattice with spin $5/2$ and spin $3/2$ respectively [32].

In 2010 Hadey K.Mohamad, studied the ferrimagnetic Ising model with nearest neighbour interactions for a square lattice and simple cubic one, using mean

field theory . Clear indication of the single – ion anisotropies on the compensation point of the mixed spin -3/2 and spin- 5/2 ferrimagnetic lattice are found [33] .

In 2011 Hadey K. Mohamad, introduced the ferrimagnetic Ising model with nearest neighbour interactions for a square lattice and simple cubic one, using mean field theory. The free energy of a mixed spin Ising ferrimagnetic model was calculated from a mean field approximation of the Hamiltonian. By minimizing the free energy, I obtained the equilibrium magnetizations and the compensation temperatures [34].

In 2012 Gulistan Mert, studied The magnetic properties of a mixed spin-1 and spin-3/2 Heisenberg ferrimagnetic system on a square lattice are investigated by using the double-time temperature-dependent Green's function technique. In order to decouple the higher order Green's functions[35].

In 2012 Zihua Xin, et al. studied The magnetization of mixed spin-1/2, 1 Ising diamond chain with antiferromagnetic spin exchange interaction has been investigated by using the Monte Carlo simulation. Magnetization behaviors with different antiferromagnetic interactions are simulated under magnetic field at low temperature[36].

In 2014 Ümüt Temizer, studied the dynamic critical behavior of the mixed spin-1 and spin-3/2 Ising system on a bilayer square lattice is studied by using the Glauber-type stochastic dynamics for both ferromagnetic/ ferromagnetic (FM/FM) and antiferromagnetic/ferromagnetic (AFM/FM) interactions in the presence of a time-varying external magnetic field[37].

In 2015 J. A. Reyes et al, obtained the magnetic properties of a ferrimagnetic mixed spin-3/2 and spin-5/2 Ising model with two crystal fields, in a longitudinal magnetic field, are studied by Monte Carlo simulations The role of the

different interactions in the Hamiltonian is explored. Depending on the region of the parameter space, we find some interesting phenomena such as compensation temperatures, and discontinuities in the magnetizations [38].

In 2018 H. Bouda1 et al, obtained The ferrimagnetic systems have been extensively investigated because of their fascinating properties. In this paper, the mixed spin-7/2 and spin-3 Ising system with periodic boundary conditions on a square lattice has been studied using the Monte Carlo simulation within the Metropolis algorithm [39].

In 2019 H. Bouda1, et al. have attracted The effects of single-ion anisotropies and an external magnetic field on the magnetization of the mixed-spin (7/2, 3/2) ferrimagnetic Ising system are investigated within Monte Carlo simulation. Under certain values of the physical parameters, multiple hysteresis loop behaviors such as double, triple, and quintuple hysteresis cycles have been observed. Particularly, the superparamagnetic phase has been shown. The ground-state phase diagrams are presented[40].

In 2019 Hadey k. mohamad & Hasan F . Alturki , investigated the magnetic phase transition and compensation point in a series of molecular – based magnetic material using the Oguchi approximation . The considrd system is a mixed spin- 3/2 and spin – 5/2 Blume – Capel Ising ferrimagnet with different single – ion anisotropies ob both simple cubic and face – centered cubic lattices respectively [41].

In 2019 Hadey K . Mohamad & Amenah Zuhair ,studied Ground – state phase diagram of mixed spin -3/2 and spin- 7/2 Ising model a study of complex $[\text{Cr}(\text{cn})_4(\mu\text{-CN})_2\text{Gd}(\text{H}_2\text{O})^4(\text{bpy})]_n.4n\text{H}_2\text{O}.1.5n\text{bpy}$, the phase transition for a molecular – based magnet , are examined using mean field method (MFM). The longitudinal magnetization can be achieved by minimizing the free energy is an

interesting function for locating and induction of spin compensation temperatures as well [42] .

In 2020 Jordana Torrico et al, studied Magnetic behavior of a ferroferrimagnetic ternary alloy $AB\rho C_{1-\rho}$ with a selective site disorder: Case study of a mixed-spin Ising model on a honeycomb lattice Phase transitions, compensation phenomenon, and magnetization of a ferroferrimagnetic ternary alloy $AB\rho C_{1-\rho}$ composed of three different kinds of magnetic ions A , B , and C with the spin magnitudes $1/2$, 1 and $3/2$ are examined within the framework of a mixed-spin Ising model on a honeycomb lattice with a selective annealed site disorder on one of its two sublattices[43].

In 2020 M. Karimou, M. Bati examined Magnetic Properties of spin-7/2 Blume-Capel Chain Under a Magnetic Field A magnetic property of the one dimensional spin-7/2 Blume-Capel model under the magnetic field has been investigated by means of transfer matrix method. Thermodynamic response functions are also obtained for varying values of reduced thermodynamic temperature and scaling magnetic field. We have seen that the crystal field strongly affects magnetic plateau mechanism[44].

In 2021 Wenhua Qin et al, recorded the exact formulations of magnetizations for a mixed spin-1/2 and spin-3/2 Blume-Capel Ising ferromagnetic model on Bethe lattice in a longitudinal magnetic field are presented. The exact expressions for sublattice magnetizations and average magnetization per site are obtained, respectively, and the temperature dependence of the magnetizations for the Bethe lattice with coordination number 4 is numerically studied [45].

1.6 Aims of this study

1. To construct a mixed spin-3 and spin-7/2 ferrimagnetic Blume – Capel (BC) Ising ground – state phase diagrams .
2. To Study seconded order phase transition for a mixed spin ferrimagnetic system using landau expansion for square and Sc lattices.
3. To examine different magnetic anisotropies of the atoms on the induction and location of ferrimagnetictn compensation temperature .
4. To investigate phase transitions within a developed mean – field method (MFM) in the study of the sublattices magnetization of the atoms constituting the proposed systems.

1.7 Thesis Outline

The outline of this thesis was arranged as follows; Chapter one presents an introduction and literature review including classification of magnetic materials. Chapter two contains the fundamentals of magnetism. The utilized model that has been solved by a developed Mean Field Approximation is included in chapter three. Chapter four is organized for results and discussion. Finally, the conclusions and future works are included in chapter five.

Chapter Two

Theory of Magnetization

2.1 Introduction

In this section, we will discuss the origin of the magnetic moment and theory of magnetic material behavior, namely the arrangement of magnetic moments with materials. This theory provide useful mathematical models for magnetic properties that include first and second order-disorder phase shifts such as Curie temperature and compensation points respectively, These models are important to give a reasonable explanation of some phenomena like the spontaneous magnetization due to the parallel arrangement of all the moments in the sample and from there it can be a non-parallel arrangement, i.e. there can be a spontaneous magnetization. Then one can discuss both of these cases and models that affect the rotating magnetic moments under different conditions [1]. Atoms contain many electrons, each electron has its own orbit and spinning about its own axis. Both kinds of a motion are a vector quantity that is associated with the magnetic moment, parallel to the axis of a spin and normal to the orbit of a motion , respectively . The magnetic moment of the atom, the vector sum of all electronic is moments, and two options arise [2].

2.2 Weiss Theory of Magnetization

In 1907 Weiss put the fundamentals of the first theory of interaction magnetic system . He was talked about cooperative ordering could be simulation by assuming that each spin was subjected to an effective field called the molecular field and it is proportional to magnetization [52]. So it is given by [13]:

$$H_m = wM \quad 2.1$$

Where w is the molecular field coefficient . The average magnetization under the effect of an external magnetic field H and a molecular field H_m is given by [15]:

$$M = \frac{Nm \int_0^\pi \exp\left(\frac{m(H+wM)}{k_B T} \cos \theta\right) \cos \theta \sin \theta d\theta}{\int_0^\pi \exp\left(\frac{m(H+wM)}{k_B T} \cos \theta\right) \sin \theta d\theta} \quad (2.2)$$

k_B is Maxwell Boltzmann constant, suppose that the parameter α is given by:

$$\alpha = \frac{m(H+wM)}{k_B T} \quad (2.3)$$

And $\cos \theta = x$, then Eq(2.2) becomes:

$$M = \frac{Nm \int_{-1}^1 x \exp(\alpha x) dx}{\int_{-1}^1 \exp(\alpha x) dx} \quad (2.4)$$

Using integration by part to solve (2.4), the solution for the numerator is:

$$\int_{-1}^1 \exp(\alpha x) x dx = \frac{1}{\alpha} (\exp(\alpha) + \exp(-\alpha)) - \frac{1}{\alpha^2} (\exp(\alpha) - \exp(-\alpha)) \quad (2.5)$$

and the integral in the denominator is calculated to be:

$$\int_{-1}^1 \exp(\alpha x) dx = \frac{1}{\alpha} |\exp(\alpha x)|_{-1}^1 = \frac{1}{\alpha} (\exp(\alpha) - \exp(-\alpha)) \quad (2.6)$$

By substituting Eqs. (2.5) and (2.6) in Eq. (2.4):

$$M = Nm \left(\frac{\exp(\alpha) + \exp(-\alpha)}{\exp(\alpha) - \exp(-\alpha)} - \frac{1}{\alpha} \right) \quad (2.7)$$

The last equation can be reduced:

$$M = Nm \left(\coth \alpha - \frac{1}{\alpha} \right) \quad (2.8)$$

The function between the parentheses is known as the Langevin function and denoted by $L(\alpha)$ So, Eq. (2.8) is put into the form as:

$$M = NmL(\alpha) \quad (2.9)$$

When $\alpha \ll 1$, the Langevin function can be expanded as Taylor series:

$$L(\alpha) = \frac{\alpha}{3} - \frac{\alpha^3}{45} \dots \quad (2.10)$$

The terms of $L(\alpha)$ other than the first one will be neglected so that Eq. (2.8) will be:

$$M = \frac{N_m}{3} \alpha \quad (2.11)$$

Since Eq. (2.3) includes M , we can solve it with respect to M , and one has:

$$M = \frac{k_B T}{mw} \alpha - \frac{H}{w} \quad (2.12)$$

The solution of Eq(2.9) can be obtained graphically. Figure 2.1 shows the curves of Eq.(2.9) and Eq.(2.12) with respect to α . Eq. (2.9) represents the Langevin function as shown by curve (a) in Figure 2.1. Let us assume that $H=0$, such that H is an external field, and the spontaneous magnetization can be produced even at the absence of the external field. In this case, Eq. (2.12) becomes a straight line (b) through the origin.

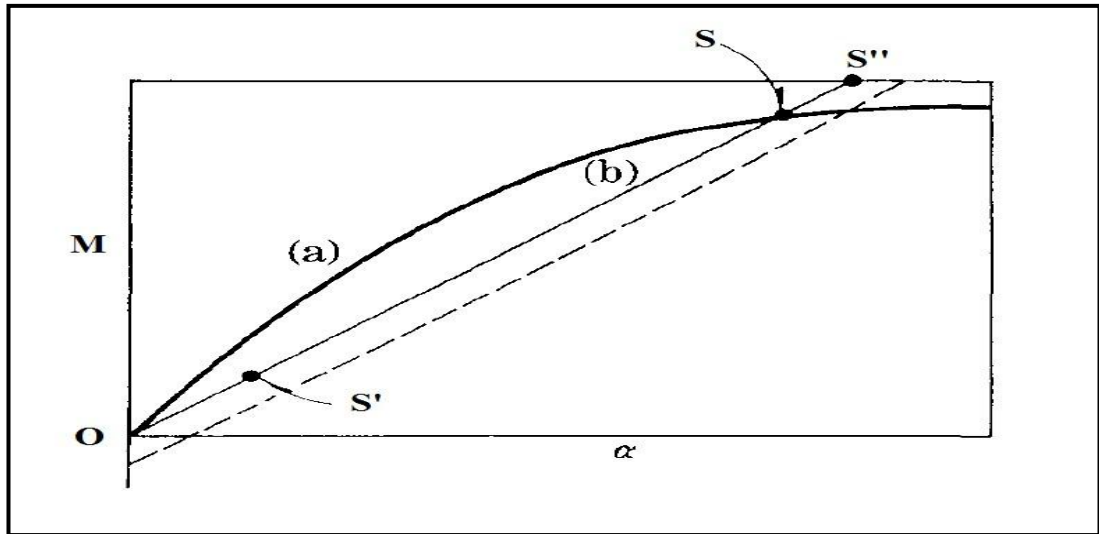


Figure 2.1: Graphical solution for spontaneous magnetization: (a) Langevin function (b) Equation (2.12) [13].

The solutions can be obtained by observing the intersection points O and S of curves (a) and (b). However, the point O produces an unstable solution, because if the magnetization has a non-zero value, such as S', near the origin, the state S' must rise along curve (b) (due to the definition of α , which entails that the state S' must always stay on the line (b)). The state of thermal equilibrium represented by curve (a) is above point S' until S' reaches S. Physically point O represents a completely random orientation of the spins. When there is some arrangement of spins by random processes, the alignment releases a non-zero molecular field, which leads to alignment that is more efficient. In contrast, point S represents a reasonable solution, because if the state changes from S to S'', the equilibrium state is always near S.

Now let us speculate the dependence of spontaneous magnetization on temperature using the graphical solution mentioned earlier. At $T=0$, the slope of the line (b) is zero, which indicates that the point S goes far to the right side, where $L(\alpha) = 1$ and $M = Nm$. This state is known as the saturation magnetization and denoted by M_S so [13]:

$$M_S = Nm \quad 2.13$$

The derivative of the Langevin function with respect to (α) is given by:

$$\frac{dM}{d\alpha} = Nm \left(\frac{\partial L(\alpha)}{\partial \alpha} \right)_{\alpha=0} = \frac{Nm}{3} \quad 2.14$$

Eq. (2.10) must be equal to the gradient of the line (b) in Eq. (2.12) at $T=T_C$, that:

$$\left(\frac{dM}{d\alpha} \right)_{\alpha=0} = \frac{K_B T_C}{mw} \quad 2.15$$

Equating Eq. (2.14) with Eq. (2.15), we have:

$$T_C = \frac{Nm^2w}{3k_B} \quad 2.16$$

So far the effect of the external field has been neglected, because the external field is usually very weak compared to the exchange field i.e. very small influence on the magnitude of spontaneous magnetization. The second term in Eq. (2.16) gives the effect of the external field, which causes a shift of line (b) in Figure 2.2 downwards and hence a shift of the point S upwards, thus the magnetization.

$$\chi = \frac{dM}{dH} = Nm \frac{\partial L(\alpha)}{\partial \alpha} \frac{\partial \alpha}{\partial H} \quad 2.17$$

Moreover, from the definition of α in Eq. (2.7), one has:

$$\frac{\partial \alpha}{\partial H} = \frac{m}{k_B T} + \frac{mw}{k_B T} \cdot \frac{dM}{dH} \quad 2.18$$

Substituting $\frac{\partial \alpha}{\partial H}$ from Eq. (2.17) and Eq. (2.18), results:

$$\chi = \frac{Nm^2 L'(\alpha)}{k_B(T - 3T_C L'(\alpha))} \quad 2.19$$

Where $L'(\alpha)$ is the differential function of $L(\alpha)$ with respect to α . At very low values of temperature $T \ll T_C$, $L'(\alpha)$ is very small that it gives a small value for the susceptibility Eq. (2.19). The susceptibility cannot be calculated without using high magnetic field. Hence, it is known as the high field susceptibility. However, when T reaches T_C , $L'(\alpha) = 1/3$ that the denominator of Eq. (2.19) tends to vanish and the susceptibility approaches infinity. At $T > T_C$, the point S' remains near the origin in Fig.(2.2), where $L(\alpha) = 1/3$, so that Eq. (2.19) becomes :

$$\chi = \frac{Nm^2 L'(\alpha)}{k_B(T - 3T_C L'(\alpha))} \quad 2.20$$

That is the susceptibility is inversely proportional to the deviation of T from T_C which is called the Curie-Weiss law. The susceptibility dependence on the temperature has been obtained as shown in Figure 2.2 [4, 13].

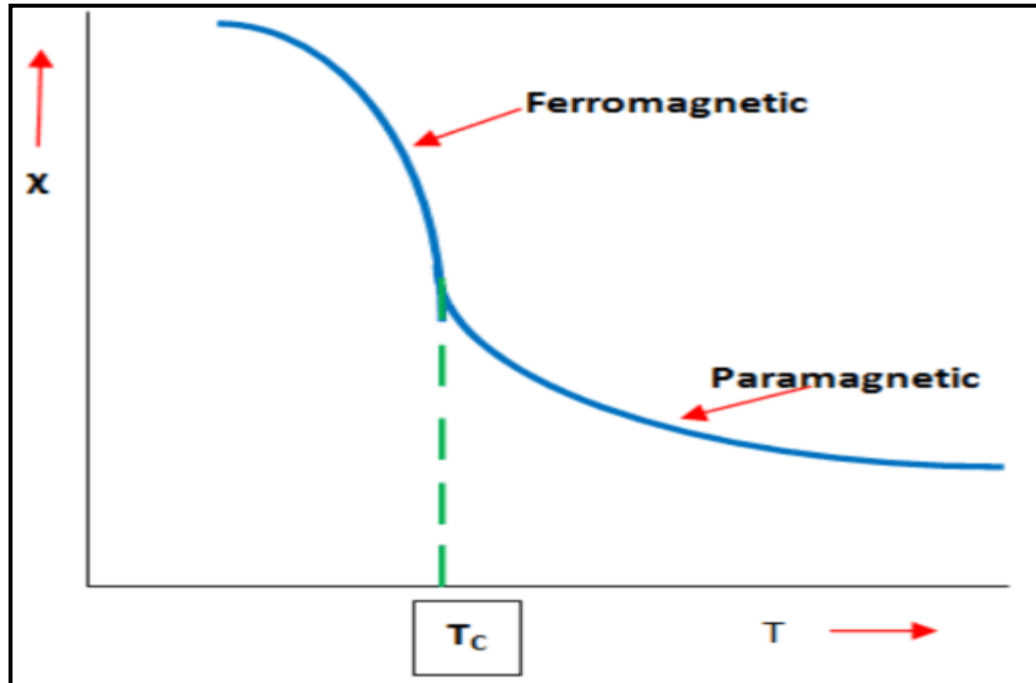


Figure2.2. Represents magnetic susceptibility near the Curie temperature [1]

2.3 Magnetic Domains

Weiss made one of the most important advances in understanding ferromagnetism in two papers published in 1906 and 1907, respectively [7]. In these papers, Wiess suggested the existence of magnetic domains in ferromagnets. These domains have a large number of atomic moments that are aligned together, typically 10^{12} to 10^{15} , so that the magnetization inside a domain has a non-zero value at the absence of any external field. However, the direction of alignment varies from domain to domain in a random manner, although certain crystallographic axes are preferred by the magnetic moments, which will become parallel with one of these equivalent magnetic easy axes [8].

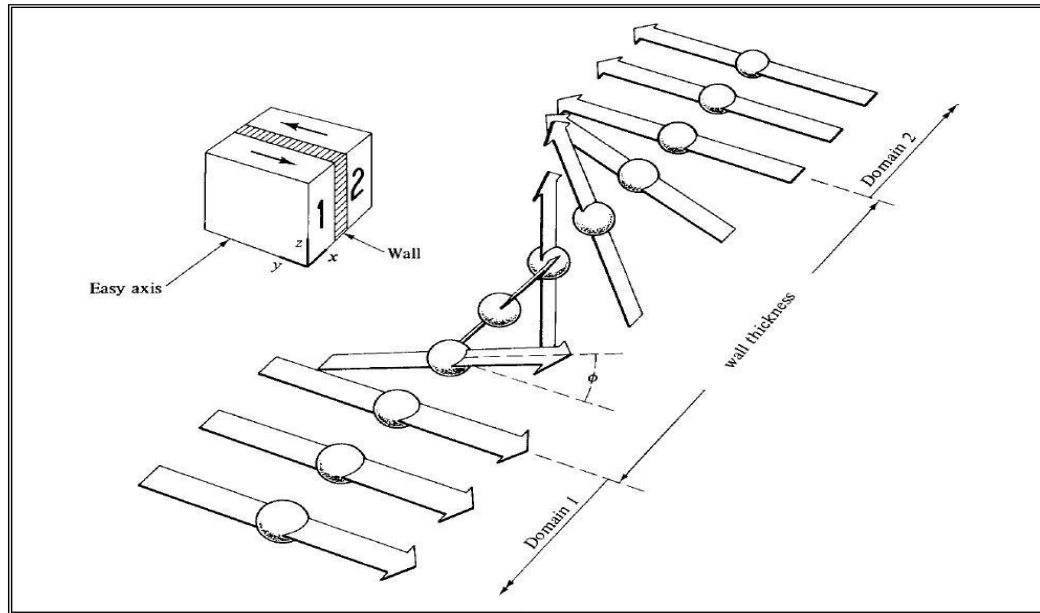


Figure 2.3: The gradual change of magnetic moment directions across the domain walls [9].

These regions are separated by thin walls called the domain walls, inside these walls the magnetization must change direction from one easy crystallographic direction to another. This change in direction does not occur abruptly, but in such a way that it changes gradually over many atoms inside the walls which means that the walls in general have a non-zero width about (10-100) nm and a definite structure. These walls are often called Bloch walls since F. Bloch made the first theoretical examination of domain walls in 1932 [9]. Figure 2.3 shows how the magnetic moments change their direction gradually within the domain wall.

As an external magnetic field is applied, the domains change shape and size by the movement of domain walls. Schematic domain structures are represented in the insets (labeled U through Z) at several points along the B-H curve in Figure 2.4.

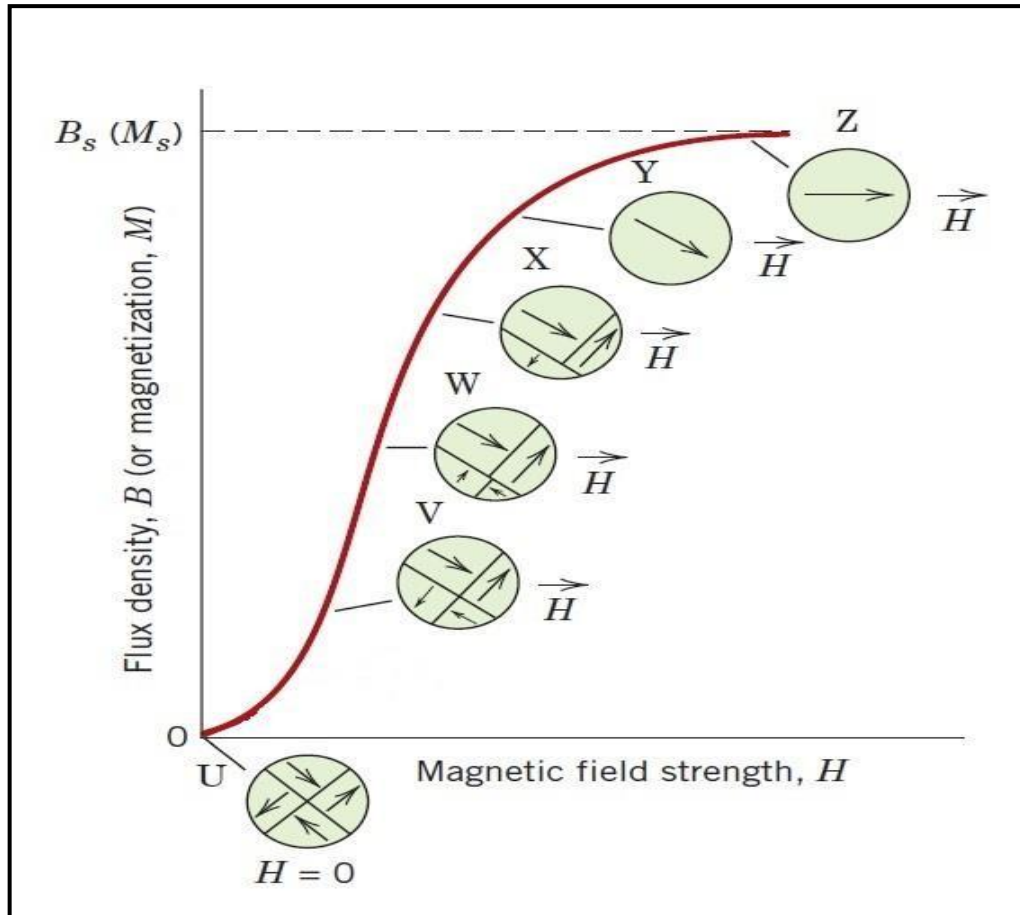


Figure 2.4: B-H behavior for an un-magnetized ferromagnetic or ferrimagnetic material [5].

Initially, the moments of the constituent domains are oriented randomly such that there is no net magnetization (M) or B field. As the external field is applied, the domains, that are oriented in direction of the applied field (or nearly aligned with the field), will grow at the expense of those which are unfavorably oriented. This growth will continue with the increasing field strength until the whole sample becomes a single domain, which is nearly aligned with the field. Saturation will occur (at Z) when this domain becomes aligned with the field [5].

At the point of saturation (S) in Figure 2.5, an external magnetic field is applied in the opposite direction, the field does not retrace its original path and a hysteresis loop will result, in which the B field lags behind the applied H field, or decreases at a lower rate. When the H field reaches zero point, the curve will have a certain

value (point R on the curve). There exists a residual B field called remanence B_r indicates that the material remains at the magnetized state in the absence of an external magnetic field.

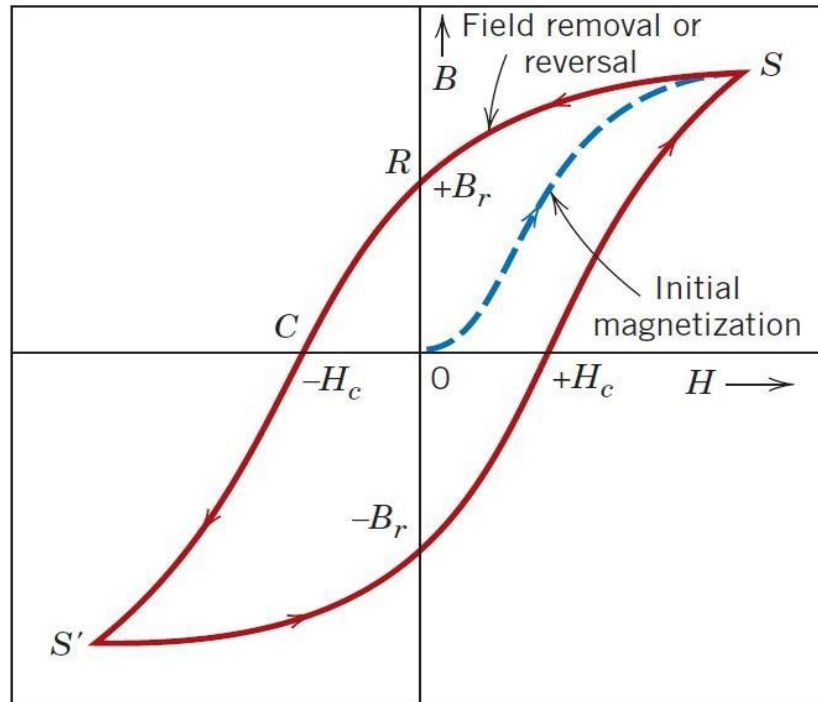


Figure 2.5: Represents the hysteresis loop [5].

To reduce the B field in the sample to zero, an H field of magnitude $-H_c$ must be applied in the opposite direction of the original field. This value of H_c is called the coercivity. By increasing the reversed magnetic field as shown in Figure 2.5 then saturation will be achieved in the opposite sense corresponds (point S'). A second reversal of the field to the point of the first saturation (point S) completes the symmetrical hysteresis loop and yield a negative remanence and positive coercivity [5, 8]. Magnetic flux density versus the magnetic field strength for a Ferromagnetic material that is subjected to forward and reverse saturations (Points S and S') Figure 2.5. The hysteresis loop is represented by the solid curve, while the dashed curve indicates the initial magnetization.

On increasing the temperature of the ferromagnetic specimen, the spontaneous magnetization starts decreasing smoothly until it vanishes at ($T=T_c$), see Figure 2.6, T_c is a specific point known as Curie temperature, indicating that the specimen undergoes a second order phase transition from ferromagnetic phase to paramagnetic phase. This transition occurs because of the thermal agitation due to the increasing in the thermal energy resulting in a random orientation of the spins [14].

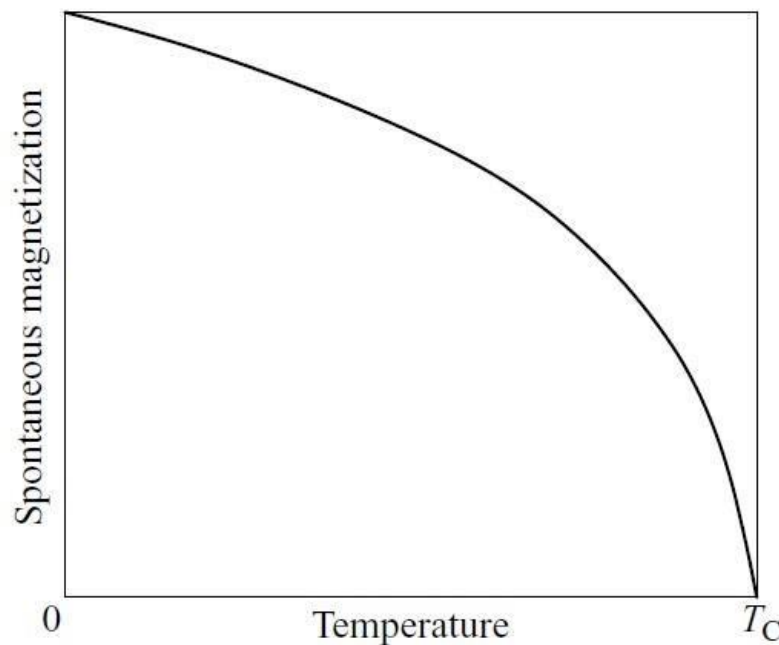


Figure 2.6: Variation of spontaneous magnetization with temperature in ferromagnetic materials [14].

2.4 Statical Distributions

Statistical mechanics treats matter as a single particle. As for most branches of physics such as (classical mechanics, atomic physics, quantum mechanics, and nuclear physics), they deal with one to hundreds of particles at one time, while statistical mechanics deals with only one mole at a time [75]. Random variables are measured and analyzed in terms of their statistical and probability properties, and the distribution function is an essential aspect of them. Although there are many possible

distribution models, only a few have gained popularity in practice, either because of desirable mathematical properties or because they apply particularly well to a part of the truth, or both[61],

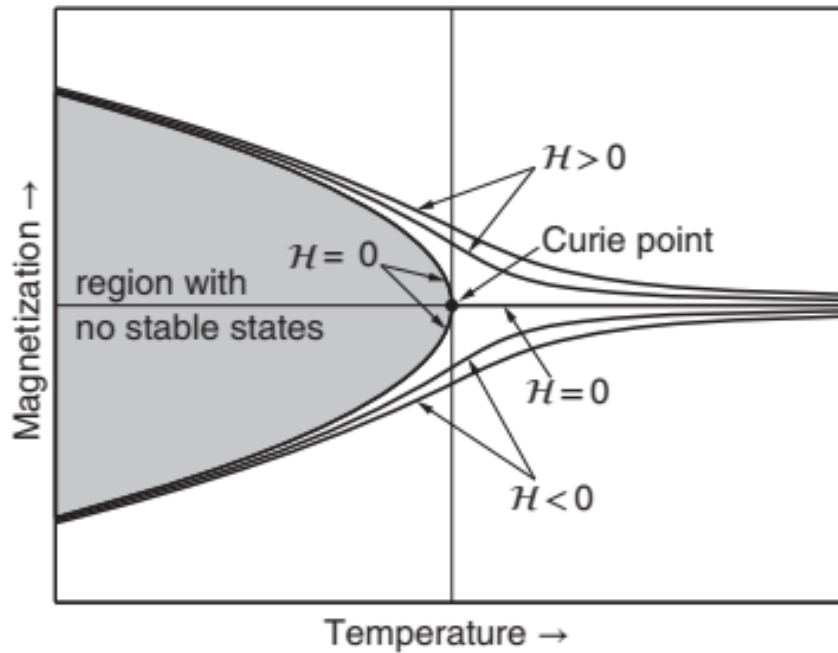


Figure 2.7 Magnetization of a Ferromagnetic System[6]

The study of thermodynamic behavior is facilitated by the small number of variables required [62]. The paramagnetic-ferromagnetic transition in magnetic materials is an important example of a second order transition. In analogy to PVT systems, we can think of magnetic materials as HMT systems, where H is the magnetic field and M is the magnetization. Figure 2.7 shows the typical dependence of M on temperature T and field H in systems with a single magnetic domain. The magnetization has two possible orientations ("up" and "down") determined by the shape of the sample and its microscopic structure. The horizontal line across the center of the figure represents states of zero magnetization ($M = 0$), points above it represent the "up" orientation

($M > 0$), and points below it represent the "down" orientation ($M < 0$). The critical point of the system is called the Curie point [6] .

2.4.1 Maxwell - Boltzmann Distribution

The Boltzmann distribution, the formula that tells us how to quantify the number of molecules in each state of a system at any temperature, is the single most significant result in all of statistical thermodynamics[71]:

$$N_i = \frac{N e^{\frac{-E_i}{kT}}}{Z} \quad (2.21)$$

Here N_i is the number of molecules in a state with energy E_i , N is the total number of molecules, k is Boltzmann's constant, a fundamental constant with the value $1.381 \times 10^{-23} \text{ J K}^{-1}$, and T is the absolute temperature. Boltzmann's constant k and the gas constant R are related by $R = kN_A$. The term in the denominator, Z , is the partition function:

$$Z = \sum_i e^{-E_i/kT} = e^{-E_0/kT} + e^{-E_1/kT} + \dots \quad (2.22)$$

where the sum is over all the states of the system. We shall have much more to say about q later, and see how it can be calculated and given physical meaning. At this stage it is just a kind of normalization factor, for it ensures that $\sum N_i = N$.

The derivation of Eq. (2.21) has a very clear conceptual basis. We imagine a stack of energy levels stacked one on top of the other, like bookshelves. Then we imagine being blindfolded and tossing balls (molecules) at shelves (energy levels), allowing them to land on every available shelf at random, with one exception. This is the condition: the total energy, E , The actual energy of the sample of matter we're trying to explain must be included in the final arrangement.

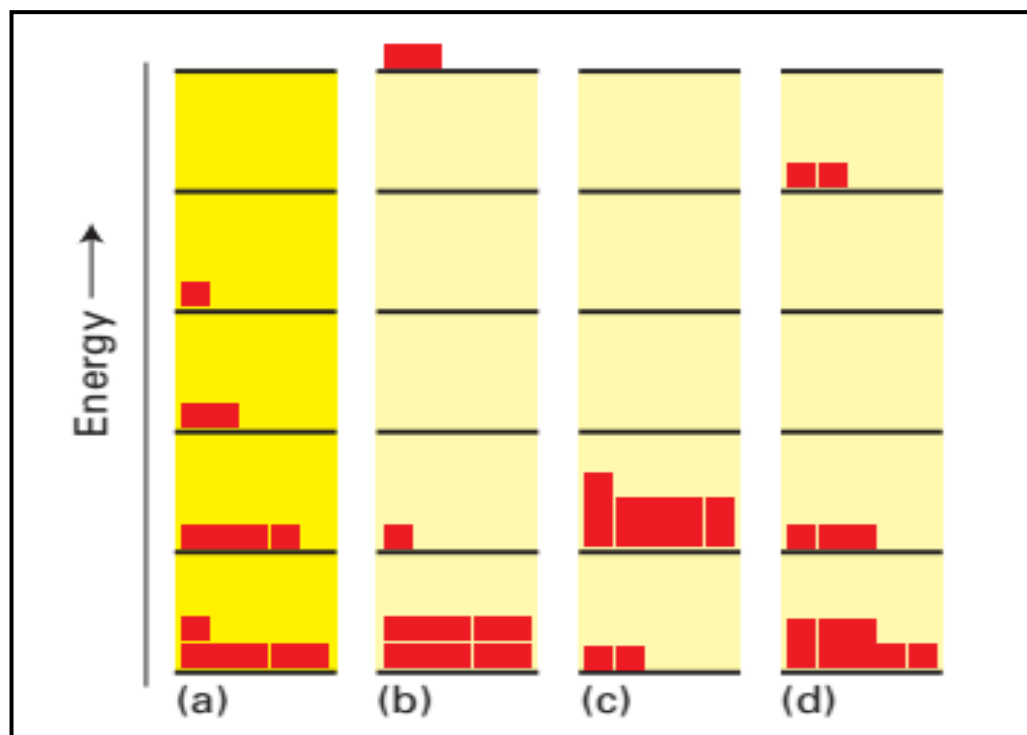


Figure 2.8 Shows the Boltzmann distribution involves imagining that the molecules of a system (the squares) are distributed at random over the available energy levels subject to the requirements that the number of molecules and the total energy is constant, and then looking for the most probable arrangement[71].

As long as the temperature is above absolute zero, no balls are allowed to land on the bottom shelf, as this will result in zero total energy. Some balls can end up on the bottom shelf, but others must end up on higher shelves in order for the total energy to be E . If we imagine tossing 100 balls at a collection of shelves, we will arrive at a single true distribution. We would end up with one true distribution if we replicate the experiment by throwing 100 balls at a collection of shelves. We will get a different but still true distribution if we repeated the experiment with the same number of balls. If we kept running the experiment, we'd end up with a variety of distributions, some of which would occur more often than others. (Figure. 2.8)

The number of ways of achieving (a) is by far the greatest, so this distribution is the most probable; it corresponds to the Boltzmann distribution. When this game is analysed mathematically, it turns out that the *most probable* distribution—the arrangement that turns up most often—is that given by eqn 22.1. In other words, the Boltzmann distribution is the outcome of blind chance occupation of energy levels, subject to the requirement that the total energy has a particular value. When we deal with too much molecules and repeat the experiment many of times, the Boltzmann distribution turns out to be very accurate, and we can use it with confidence for all typical samples of matter. The simplest application of the Boltzmann distribution is to calculate the relative numbers of molecules in two states separated in energy by ΔE . Suppose the energies of the two states are E_1 and E_2 , then from eq 2.21 we can write:

$$\frac{N_2}{N_1} = \frac{e^{-E_2/KT}}{e^{-E_1/KT}} = e^{-(E_2 - E_1)/KT} = e^{-\Delta E/KT} \quad (2.23)$$

where $\Delta E = E_2 - E_1$. This important result tells us that *the relative population of the upper state decreases exponentially with its energy above the lower state*. In this expression, the energy difference is in joules. If the energy difference is given in joules (or kilojoules) per mole, we simply use the gas constant in eqn 22.3 in place of Boltzmann's constant (because $R = KN_A$)[71].

2.4.2 Quantum Distributions

The Bose-Einstein distribution describes systems of similar bosons, such as electrons and ^3He atoms, while the Fermi-Dirac distribution describes systems of identical fermions, such as ^4He atoms. Fermi-Dirac and Bose-Einstein distributions can be found using the same methods used to derive the Maxwell distribution for

velocities. We consider systems of identical N particles with a total energy of E . The goal of our exercise is to determine how many different ways the particles can be arranged between intervals. The numbers describe the particle distribution. $n_1, \dots, n_j, \dots$, where n_j is the number of particles in the interval j . The distribution is constrained by the conditions that:

$$N = \sum_j n_j \quad \text{and} \quad E = \sum_j n_j \epsilon_j \quad (2.24)$$

The equilibrium distributions for both fermions and bosons are obtained by assuming that The distribution of particles in thermal equilibrium is given by the numbers n_1, n_j , that maximize the number of arrangements consistent with the values of N and E [70].

2.4.2 a Bose - Einstein Distribution

The number of ways that n_j particles can be arranged among K_j single-particle states, when any number of bosons are allowed in each state, is needed to find the Bose - Einstein distribution.



Figure 2.9 A Sequence of White and Black Objects shows distribution of particles energy levels [70].

This number is referred to as $w.f.(n_j)$. Finding it is the same as figuring out how many different forms there are for N white objects (bosons) to be put in M boxes (states) without distinguishing the objects from each other. The combinatorial

problem is solved by imagining that we have N distinct white objects and $M - 1$ distinct black objects arranged along a line, as depicted in Figure 2.9.

The black artifacts are thought to be partitions between adjacent boxes. A box, such as box number 2 in the figure, may be empty. M boxes are created by the $M - 1$ walls. The number of ways to arrange n distinct objects is $n!$ so the number of ways to arrange the $N + M - 1$ black and white objects along the line is $(N + M - 1)!$. Since the boxes can be distinguished based on their location, along the line, rearranging the $M - 1$ black objects has no effect on our ability to identify them. As there are $(M - 1)!$ ways in which they can be arranged, we divide by $(M - 1)!$. Since the white objects are distinct, there are $N!$ ways of arranging them. To obtain the number of arrangements when the objects are not distinguished from each other, we divide by $N!$. Thus: *The number of ways that N white objects can be placed in M boxes without distinguishing the object from each other is $(N + M - 1)! / (N!(M - 1)!)$ [70].*

2.4.2b Fermi - Dirac Distributions

Let K_j represent the number of single-particle states in interval j . To find the Fermi-Dirac distribution, we need to determine the number of ways that n_j particles can be arranged among K_j states with no more than one particle in each single-particle state. Represent the number of ways by $w_f(n_j)$. Finding $w_f(n_j)$ is equivalent to the combinatorial problem of finding the number of ways of choosing n_j objects (fermions) from a collection of K_j objects (states) without regard to order. The number of ways of choosing M objects from a collection of N distinct objects without regard to order is given by the binomial coefficient $N! / (M!(N - M)!)$. By replacing the N in this by K_j and the M by n_j , we obtain the number of ways that n_j identical particles can be arranged in K_j single-particle states [14].

CHAPTER THREE

Mean - Field Approximation and Phase Transition Of The System

3.1 Introduction

Due to the great technological applications, research has recently been directed to the investigations of magnetic phase transitions of the mixed spin Ising systems. In two-dimension, the exact critical temperature T_C for the square lattice Ising model was obtained by Kramers and Wannier. Other exact results, including T_C , have been found for honeycomb and triangular lattices, respectively[45]. For other lattices and higher dimensions there is no exact calculation of T_C , however, various forms of molecular field theory have been applied and improved upon. In magnetism, the molecular or mean-field approximation(MFA) originally used by Pierre Weiss was very successful at showing the transition to a magnetically ordered state for Heisenberg and Ising models at a non-zero transition temperature T_C [46]. However, the standard mean-field approach can be shown to be equivalent to having each site interacting equally with all other sites; its prediction of critical temperature is not very accurate. Physically, having a particular spin interacting equally with all others of the system ignores both the presence of a finite correlation length and the strong fluctuations near T_C . Mean-field theory has other faults; it can predict a phase transition at finite temperature in one-dimension Ising model, an impossibility not present in the exact solution.

3.2 Ising Model in the Mean-Field Theory

Because of its importance, the mean-field approximation has played an important role for the description of cooperative phenomena. In the mean-field theory, it is assumed that each spin doesn't interact directly with its nearest neighbours, but with a mean field, which follows from the mean orientation of the

neighboring spins. So, the Hamiltonian of a system having spin-1/2 in a magnetic field is [29].

$$H = -\sum_{i=1}^N \sum_{j=1}^N J_{ij} S_i S_j - h \sum_{i=1}^N S_i \quad (3.1)$$

i.e., J_{ij} is the exchange interaction between spins at sites i and j .

Since the exchange interaction decreases rapidly with distance, we need to consider only nearest neighbors in the lattice. It is assumed that the interaction is equal for every pair of sites, that, $J_{ij} = J_{jl} = \dots = J$, thus, by the use of the following identity:

$$< S_i S_j > = S_i < S_j > + < S_i > S_j - < S_i > < S_j > + (S_i - < S_i >)(S_j - < S_j >) \quad (3.2)$$

where the average values $< S_i >$ do not depend on the index i due to translational invariance. So, the exact interaction (Eq.(3-2), in the absence of magnetic field, $h = 0$, becomes,

$$H = -J \sum_{i,j} S_i < S_j > + < S_i > S_j - < S >^2 + (S_i - < S >)(S_j - < S >) \quad (3.3)$$

Since each central spin S_i with neighbour S_j is also a neighbouring spin of the central spin S_j , the values of the first two sums are identical. It is mentioning note, there are exactly $\left(\frac{zN}{2}\right)$ different pairs: $\left(\frac{z}{2}\right)$ different pairs belong to each spin $S_i, i = 1, \dots, N, \frac{z}{2}$

Now, Eq.(3-3) becomes:

$$H\{S_1, S_2, \dots, S_N\} = \frac{-Jz}{2} < S > \cdot 2 \sum_{i=1}^N S_i + J \frac{zN}{2} < S >^2 - J \sum_{i,j} (S_i - < S >)(S_j - < S >)$$

hence,

$$H\{S_1, S_2, \dots, S_N\} = -Jz \langle S \rangle \sum_{i=1}^N S_i + J \frac{zN}{2} \langle S \rangle^2 - J \sum_{i,j} (S_i - \langle S \rangle)(S_j - \langle S \rangle) \quad (3.4)$$

So far this expression is still exact. The first term just has the form mentioned in the beginning, while the second term represents a constant expectation value which no longer depends on a special orientation of the spins. Finally, the last term contains the spin fluctuations, i.e., the deviations of a certain spin from its mean orientation. The mean-field approximation corresponds to neglecting this term. Thus, we have the effective interaction, that[29]:

$$H^{m.f} \{S_1, S_2, \dots, S_N\} = -Jz \langle S \rangle \sum_{i=1}^N S_i + J \frac{zN}{2} \langle S \rangle^2 \quad (3.5)$$

since,

$$Z = \sum_{S_1} \sum_{S_2} \dots \sum_{S_N} e^{-\beta H^{m.f}} \quad (3.6)$$

Now, substituting Eq.(3-5) in Eq.(3-6), one has:

$$Z = e^{-t \frac{zN}{2} \langle S \rangle^2} [2 \cosh\{zt \langle S \rangle + H\}]^N \quad (3.7)$$

with,

$$t = \beta J ; H = \beta h$$

where, h stands for an external magnetic field.

3.2.1 Free Energy

The free energy is proportional to the logarithm of the partition function as,

$$G = -k_B T \ln Z \quad (3.8)$$

substituting Eq.(3-7) in Eq.(3-8), we get:

$$G(N, T, H, \langle S \rangle) = J \frac{zN}{2} \langle S \rangle^2 - Nk_B T \ln[2 \cosh(zt \langle S \rangle + H)] \quad (3.9)$$

3.2.2 Spontaneous Magnetization

In this item, we can directly give an expression for the magnetization of the solid, as follows:

$$M(H, T) = -\beta \left(\frac{\partial G}{\partial H} \right)_T \quad (3.10)$$

Substituting Eq.(3-9) in Eq.(3-10), that:

$$M(H, t, N, \langle S \rangle) = N \tanh(zt \langle S \rangle + H) \quad (3.11)$$

The spontaneous magnetization is obtained by setting the applied field $h = 0$, giving a transcendental equation for the order parameter, that:

$$\langle S \rangle \equiv m = \tanh(ztm) \quad (3.12)$$

The last equation stands for the reduced magnetization in the absence of magnetic field. The mean-field approximation is to assume that all the other spins are of equal influences, however distant they are. Thus, for simplicity, we can write down the Hamiltonian of a system having spin-1/2 in a magnetic field, as follows:

$$H = -JS_i N \sum_{j=1}^N S_j - h \cdot NS_i \quad (3.13)$$

Also, it could be written that, $\sum_j S_j \rightarrow z \langle S_j \rangle$ then,

$$H = -JS_i z \langle S_j \rangle - hS_i \quad (3.14)$$

This is an idea of approximation in the mean-field theory, where z stands for a coordination number. Using Maxwellian-Boltzmann distribution, one has the reduced magnetization[47]:

$$\langle S_i \rangle \equiv \langle S_j \rangle = \frac{\sum S_i e^{-\beta H}}{Z} \quad (3.15)$$

hence,

$$m = \tanh(tzm + H) \quad (3.16)$$

The magnitude of m obtained by solving(3-16) is shown in Fig.(3-1), plotted as a function of T . The order parameter grows rapidly below T_C , reaching almost unity at $\frac{1}{3}T_C$. One of the characteristic features of the mean-field approximation is the total lack of order when $T > T_C$; the solid is effectively in a paramagnetic state in spite of the interactions between spins.

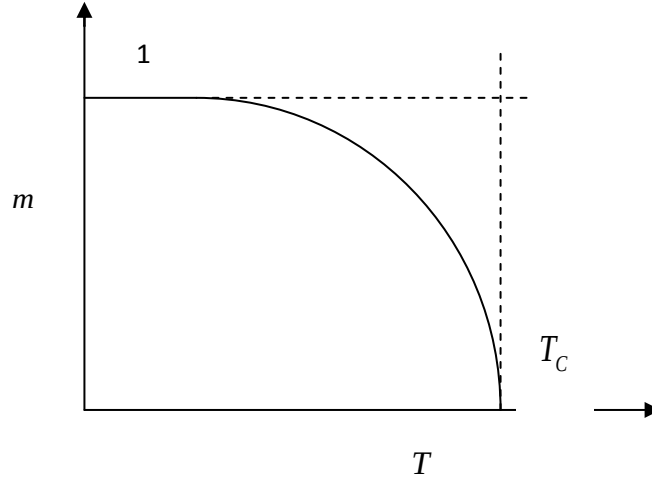


Figure (3.1): Variation of the order parameter m with the absolute temperature T . [75]

3.3 Mean-Field of A Mixed Spin Ising System

The central idea of the mean-field theory is very simple : we treat the nearest neighbour Ising model in zero field on a lattice containing two sublattices A,B having N sites , each site having z nearest neighbours . The introduction of uniaxial crystal-field effects in the whole mixed-spin system requires a spin representation larger than $(1/2)$. The spin-one Ising model with a crystal-field interaction is often called the Blume-Capel(BC) model[47,48], which is described for a mixed-spin system consisting of two types of atoms A and B by the following Hamiltonian[49],

$$H = -J \sum_{i,j} s_i^A s_j^B - D_A \sum_i (s_i^A)^2 - D_B \sum_j (s_j^B)^2 \quad (3-17)$$

D_A, D_B are the anisotropies acting on the spins for A-atoms and spins for B-atoms respectively. J is the nearest-neighbor exchange interactions. Maxwell-Boltzmann statistics are appropriate because the magnetic systems we consider consist of localized, and hence distinguishable, spins will be in the classical regime. Thus, the expectation value of the spin variable at the sites i or j is given by[50],

$$\langle m_{i/j} \rangle = \frac{1}{Z} \text{Tr} s_{i/j} e^{-\beta H} \quad (3-18)$$

with ,

$$Z = \text{Tr} e^{-\beta H} \quad (3-19)$$

where Tr means the sum over allowed states of the system . Here, $\beta = \frac{1}{k_B T}$.

3.4The Proposed Mixed-Spin System

Now let us substitute the Hamiltonian of the system, consisting of spins s_i^A taking the values of $\pm 3, \pm 2, \pm 1$, and spins s_j^B taking the values of $\pm 7/2, \pm 5/2, \pm 3/2, \pm 1/2$, in the equation(3-18), that one has :

$$m_{s_i^A=3} = \frac{1}{2} \frac{6 \sinh(3\beta\lambda_A) + 4e^{-5\beta D_A} \sinh(2\beta\lambda_A) + 2e^{-8\beta D_A} \sinh(\beta\lambda_A)}{\cosh(3\beta\lambda_A) + e^{-5\beta D_A} \cosh(2\beta\lambda_A) + e^{-8\beta D_A} \cosh(\beta\lambda_A) + 0.5e^{-9\beta D_A}} \quad (3-20)$$

with, $\lambda_A = zJm_B$

where z is the nearest-neighbour coordination number of the lattice ,

$$m_{s_j^B=7/2} = \frac{1}{2} \frac{7 \sinh(3.5\beta\lambda_B) + 5e^{-6\beta D_B} \sinh(2.5\beta\lambda_B) + 3e^{-10\beta D_B} \sinh(1.5\beta\lambda_B) + e^{-12\beta D_B} \sinh(0.5\beta\lambda_B)}{\cosh(3.5\beta\lambda_B) + e^{-6\beta D_B} \cosh(2.5\beta\lambda_B) + e^{-10\beta D_B} \cosh(1.5\beta\lambda_B) + e^{-12\beta D_B} \cosh(0.5\beta\lambda_B)} \quad (3-21)$$

where $\lambda_B = zJm_A$.

3.5 Bogoliubov Inequality

Evaluate free energy of the system ($S_i^A = 3$, $S_j^B = 7/2$) based on Bogoliubov inequality. A systematic way of deriving the mean-field theory for a given microscopic Hamiltonian is to start from the Bogoliubov inequality:

$$G \leq \Phi = G_o + \langle H - H_o \rangle_o \quad (3-22)$$

where G is the free energy of the system , H_o a trial Hamiltonian depending on variational parameters , G_o the corresponding free energy ,and $\langle \dots \rangle_o$ denotes an average taken in the ensemble defined by H_o . The mean-field free energy is then defined by minimizing F with respect to the variational parameters $\lambda_{A/B}$,that this gives the best possible approximation to the true free energy for a given choice of H_o , since the inequality (Eq.(3-24))insists that the mean-field free energy cannot fall below the true free energy. In this work we consider one of the simplest possible choices of H_o , as:

$$H_o = -\sum_i [\lambda_A s_i^A + \gamma_A (s_i^A)^2] - \sum_j [\lambda_B s_j^B + \gamma_B (s_j^B)^2] \quad (3-23)$$

with,

S_i^A taking the values of spins for A-atoms, and S_j^B taking the values of spins for B-atoms. Where λ_A , λ_B , are the variational parameters related to the two different spins and the anisotropies of two-sublattices considered respectively .Then,the approximated free energy can be obtained by minimizing the right side of equation (3-22) with respect to variational parameters mentioned above. Thus, one can express Eq.(3-22) as :

$$\begin{aligned}
 \varphi = & -\frac{k_B T}{2} \{ \ln[2e^{9D_A/k_B T} \cosh(3\lambda_A/k_B T) + 2e^{4D_A/k_B T} \cosh(2\lambda_A/k_B T) + 2e^{D_A/k_B T} \cosh(\lambda_A/k_B T) + 1] \\
 & + \ln[2e^{\frac{49}{4}D_B/k_B T} \cosh(\frac{7}{2}\lambda_B/k_B T) + 2e^{\frac{25}{4}D_B/k_B T} \cosh(\frac{5}{2}\lambda_B/k_B T) + 2e^{\frac{9}{4}D_B/k_B T} \cosh(\frac{3}{2}\lambda_B/k_B T) \\
 & + 2e^{\frac{1}{4}D_B/k_B T} \cosh(\frac{1}{2}\lambda_B/k_B T)] \} + \frac{1}{2} z J m_A m_B
 \end{aligned}
 \tag{3.24}$$

where N is the total number of sites of lattice and $\varphi = \frac{\phi}{N} \equiv g$. Minimizing this expression with respect to λ_A and λ_B gives self-consistent expressions for the mean-field (as indicated in Eqs.(3.20),(3.21)):

3.6 Magnetic Phase Transitions

A phase transition is signaled by a singularity in a thermodynamic potential such as the free energy. If there is a finite discontinuity in one or more of the first derivatives of the appropriate thermodynamic potential the transition is termed first-order. For a magnetic system the free energy is the appropriate potential with a discontinuity in the magnetization showing that the transition is first-order. For a magnetic system the free energy defined by Eq.(3-8), is appropriate potential with discontinuity in the magnetization showing that the transition is first order. If the first derivatives are continuous but second derivatives are discontinuous or infinite the transition will be described as higher order, continuous, or critical. This type of transition, corresponds to a divergent susceptibility, is termed second-order phase transition. This section will be shown in Landau theory based on some assumptions.

3.6.1 Landau Theory

Landau theory is based on very simple assumptions, yet it not only predicts a phase transition but allows reproduction of the mean-field exponents showing very clearly how they depend on the symmetry of the order parameter. Landau assumed

that the free energy can be expanded as a power series in the order parameter m_A , that[51]:

$$g = g_0 + am_A^2 + bm_A^4 + \dots \quad (3-25)$$

For a mixed spin-3 and spin-7/2 Ising model for any value of parameters, it undergoes a second-order transition that some features of the phase diagram may be obtained analytically. To determine the second-order transition lines, we need to expand equations of free energy and sublattices magnetizations of the system mentioned above(Eqs.(3-20),(3-21),(3-26)). Thus, the coefficients g_0 and a are given by:

$$g_0 = -\frac{1}{2\beta} \ln\{(x_1 + x_2 + x_3 + 1)(y_1 + y_2 + y_3 + y_4)\} \quad (3-26)$$

And

$$a = -\frac{1}{2\beta} \left\{ \frac{t^4}{32} \left(\frac{9x_1 + 4x_2 + x_3}{x_1 + x_2 + x_3 + 1} \right) \left(\frac{49 + 25z_{b1} + 9z_{b2} + z_{b3}}{z_{b1} + z_{b2} + z_{b3} + 1} \right)^2 \right. \\ \left. + \frac{t^2}{8} \left(\frac{49y_1 + 25y_2 + 9y_3 + y_4}{y_1 + y_2 + y_3 + y_4} \right) \right\} + \frac{Jzt}{8} \left(\frac{49 + 25z_{b1} + 9z_{b2} + z_{b3}}{z_{b1} + z_{b2} + z_{b3} + 1} \right) \quad (3.27)$$

Where;

$$x_1 = 2e^{9\beta D_A}; x_2 = 2e^{4\beta D_A}; x_3 = 2e^{\beta D_A}$$

$$y_1 = 2e^{\frac{49}{4}\beta D}$$

and

$$z_{b1} = e^{-6\beta D}$$

where $\beta = \frac{1}{k_B T}$, and $z(z=4,6)$, the nearest-neighbor coordination number of a square lattice.

The second order phase transition line is then determined by $a=0$ and $b>0$. It is worth mentioning that Eq.(3-27) could be evaluated both Ferromagnetic phase stability limit ($J>0$) and Ferrimagnetic one ($J<0$)[52]. It is worth to note that the ferrimagnetic case shows the signs of sublattice magnetizations are different, and there may be a compensation point, at which the total longitudinal magnetization per site[53], that:

$$M = \frac{1}{2}(m_A + m_B) \quad (3-28)$$

is equal to zero, but($m_A = -m_B \neq 0$).

3.7 Evaluation of Ground-State Phase Diagram

The mixed spin-3 and spin-7/2 Blume-Capel Ising model expose sixteen phases with various values of $\{m_A, m_B, K_A, K_B\}$, i.e., the ordered ferrimagnetic phases:

$$\begin{aligned} O_1 &\equiv \{-3, \frac{7}{2}, 9, \frac{49}{4}\}, or, O_1 \equiv \{3, -\frac{7}{2}, 9, \frac{49}{4}\}, O_2 \equiv \{-2, \frac{7}{2}, 4, \frac{49}{4}\}, or, O_2 \equiv \{2, -\frac{7}{2}, 4, \frac{49}{4}\}, \\ O_3 &\equiv \{-1, \frac{7}{2}, 1, \frac{49}{4}\}, or, O_3 \equiv \{1, -\frac{7}{2}, 1, \frac{49}{4}\}, O_4 \equiv \{-3, \frac{5}{2}, 9, \frac{25}{4}\}, or, O_4 \equiv \{3, -\frac{5}{2}, 9, \frac{25}{4}\}, \\ O_5 &\equiv \{-2, \frac{5}{2}, 4, \frac{25}{4}\}, or, O_5 \equiv \{2, -\frac{5}{2}, 4, \frac{25}{4}\}, O_6 \equiv \{-1, \frac{5}{2}, 1, \frac{25}{4}\}, or, O_6 \equiv \{1, -\frac{5}{2}, 1, \frac{25}{4}\}, \\ O_7 &\equiv \{-3, \frac{3}{2}, 9, \frac{9}{4}\}, or, O_7 \equiv \{3, -\frac{3}{2}, 9, \frac{9}{4}\}, O_8 \equiv \{-2, \frac{3}{2}, 4, \frac{9}{4}\}, or, O_8 \equiv \{2, -\frac{3}{2}, 4, \frac{9}{4}\}, \\ O_9 &\equiv \{-1, \frac{3}{2}, 1, \frac{9}{4}\}, or, O_9 \equiv \{1, -\frac{3}{2}, 1, \frac{9}{4}\}, O_{10} \equiv \{-3, \frac{1}{2}, 9, \frac{1}{4}\}, or, O_{10} \equiv \{3, -\frac{1}{2}, 9, \frac{1}{4}\}, \\ O_{11} &\equiv \{-2, \frac{1}{2}, 4, \frac{1}{4}\}, or, O_{11} \equiv \{2, -\frac{1}{2}, 4, \frac{1}{4}\}, O_{12} \equiv \{-1, \frac{1}{2}, 1, \frac{1}{4}\}, or, O_{12} \equiv \{1, -\frac{1}{2}, 1, \frac{1}{4}\}, \end{aligned}$$

and disordered phases are,

$$D_1 \equiv \{0, 0, 0, \frac{49}{4}\}, D_2 \equiv \{0, 0, 0, \frac{25}{4}\}, D_3 \equiv \{0, 0, 0, \frac{9}{4}\}, D_4 \equiv \{0, 0, 0, \frac{1}{4}\}.$$

where the parameters K_A and K_B are defined as:

$$K_A = \langle (s_i^A)^2 \rangle, \quad K_B = \langle (s_j^B)^2 \rangle \quad (3.29)$$

Now let us evaluate the corresponding ground-state energies per site for these phases

as follows by using Gibbs rule [19-71]:

$$U_{O_1} = -\frac{21z|J|}{4} - \frac{9}{2}D_A - \frac{49}{8}D_B \quad (3.30)$$

$$U_{O_2} = -\frac{7z|J|}{2} - 2D_A - \frac{49}{8}D_B \quad (3.31)$$

$$U_{O_3} = -\frac{7z|J|}{4} - \frac{1}{2}D_A - \frac{49}{8}D_B \quad (3.32)$$

$$U_{O_4} = -\frac{15z|J|}{4} - \frac{9}{2}D_A - \frac{25}{8}D_B \quad (3.33)$$

$$U_{O_5} = -\frac{5z|J|}{2} - 2D_A - \frac{25}{8}D_B \quad (3.34)$$

$$U_{O_6} = -\frac{5z|J|}{4} - \frac{1}{2}D_A - \frac{25}{8}D_B \quad (3.35)$$

$$U_{O_7} = -\frac{9z|J|}{4} - \frac{9}{2}D_A - \frac{9}{8}D_B \quad (3.36)$$

$$U_{O_8} = -\frac{3z|J|}{2} - 2D_A - \frac{9}{8}D_B \quad (3.37)$$

$$U_{O_9} = -\frac{3z|J|}{4} - \frac{1}{2}D_A - \frac{9}{8}D_B \quad (3.38)$$

$$U_{O_{10}} = -\frac{3z|J|}{4} - \frac{9}{2}D_A - \frac{1}{8}D_B \quad (3.39)$$

$$U_{O_{11}} = -\frac{1z|J|}{2} - 2D_A - \frac{1}{8}D_B \quad (3.40)$$

$$U_{O_{12}} = -\frac{1z|J|}{4} - \frac{1}{2}D_A - \frac{1}{8}D_B \quad (3.41)$$

$$U_{D_1} = -\frac{49}{8}D_B \quad (3.42)$$

$$U_{D_2} = -\frac{25}{8}D_B \quad (3.43)$$

$$U_{D_3} = -\frac{9}{8}D_B \quad (3.44)$$

$$U_{D_4} = -\frac{1}{8}D_B \quad (3.45)$$

Chapter Four

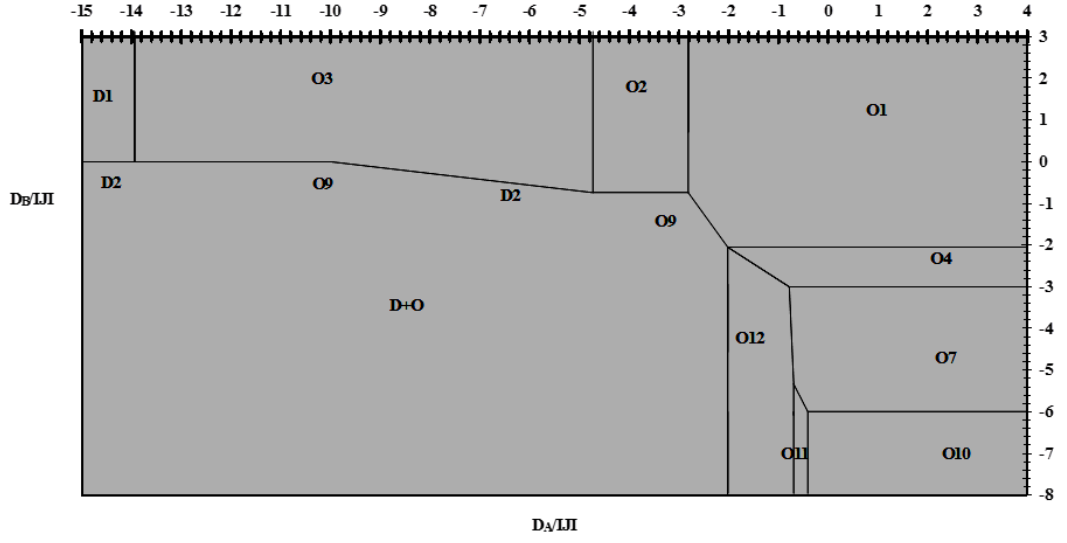
RESULTS AND DISCUSSIONS

4.1 Introduction

In recent years, a number of experimental works in the field of molecular magnetic materials has been interested. These materials are considered as molecular-based magnetic compounds which play an important role on the enhancement of the storage applications and the density speed, also, on the variations of the magnetization under the effects of both the temperature and the magnetic crystal fields of the mixed spin-3 and spin-7/2 Blume-Capel Ising system[39,40]. The obtained magnetic properties of this system have been studied to clarify and support some of the characteristic behaviors for the compounds $Gd_2O_2S:Ln^{3+}$ ($Ln = Eu, Tb$)[55,56]. It has been reported the preparation of materials: $Gd_2O_2S: Eu^{3+}$, and $Gd_2O_2S: Tb^{3+}$, respectively, through a facile solvothermal process by subsequent heat treatment process. It contains the gadolinium (Gd) element, by terbium (Tb) atoms which are coupled ferrimagnetically, the electronic configuration for $Gd : [Xe]4f^7 5d^1 5S^2$ and $Tb : [Xe]4f^6 5d^1 5S^2$, it satisfies that (Gd) holds spin-7/2 and spin-3 for (Tb), respectively[39,56]. Theoretical studies of mixed Ising systems have been intensively investigated as simple models that can show ferrimagnetic behavior. It is worth to note that the ground-state phase diagrams are useful to check the reliability of the numerical results for these diagrams at finite temperature and allow exploring regions where important magnetic behaviors could arise[54-66].

4.2 Ground-State Phase Diagram of the System

From equations (i.e., Eqs.(3.30)-(3.45)), one can compare the energies to create the ground-state phase diagram of the system with $z = 4, 6$, as shown In Figures.(4.1),(4.2), respectively.



Figure(4.1): Ground state phase diagram of the considered model with the 4 nearest neighbors and different crystal fields D_A and D_B . The ordered and disordered phase $O_1, O_2, O_3, O_4, O_7, O_9, O_{10}, O_{11}, O_{12}, D_1, D_2$, and $(D+O)$: O_5, O_6, O_8, D_3, D_4 , are separated by thin lines, respectively.

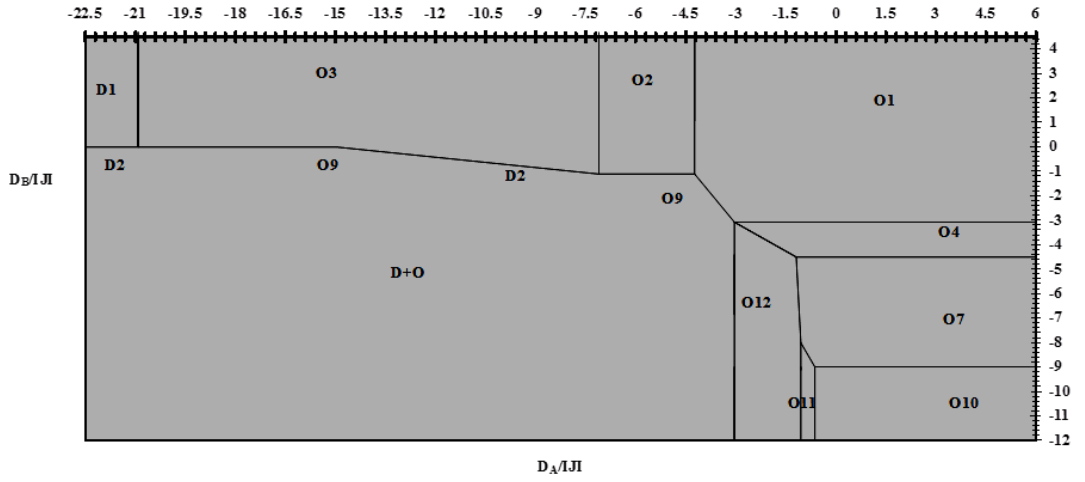


Fig.(4.2): Ground state phase diagram of the considered model with the 6 nearest neighbors and different crystal fields D_A and D_B . The ordered and disordered phases:

$O_1, O_2, O_3, O_4, O_7, O_9, O_{10}, O_{11}, O_{12}, D_1, D_2$, and $(D+O)$: O_5, O_6, O_8, D_3, D_4 , are separated by thin lines, respectively.

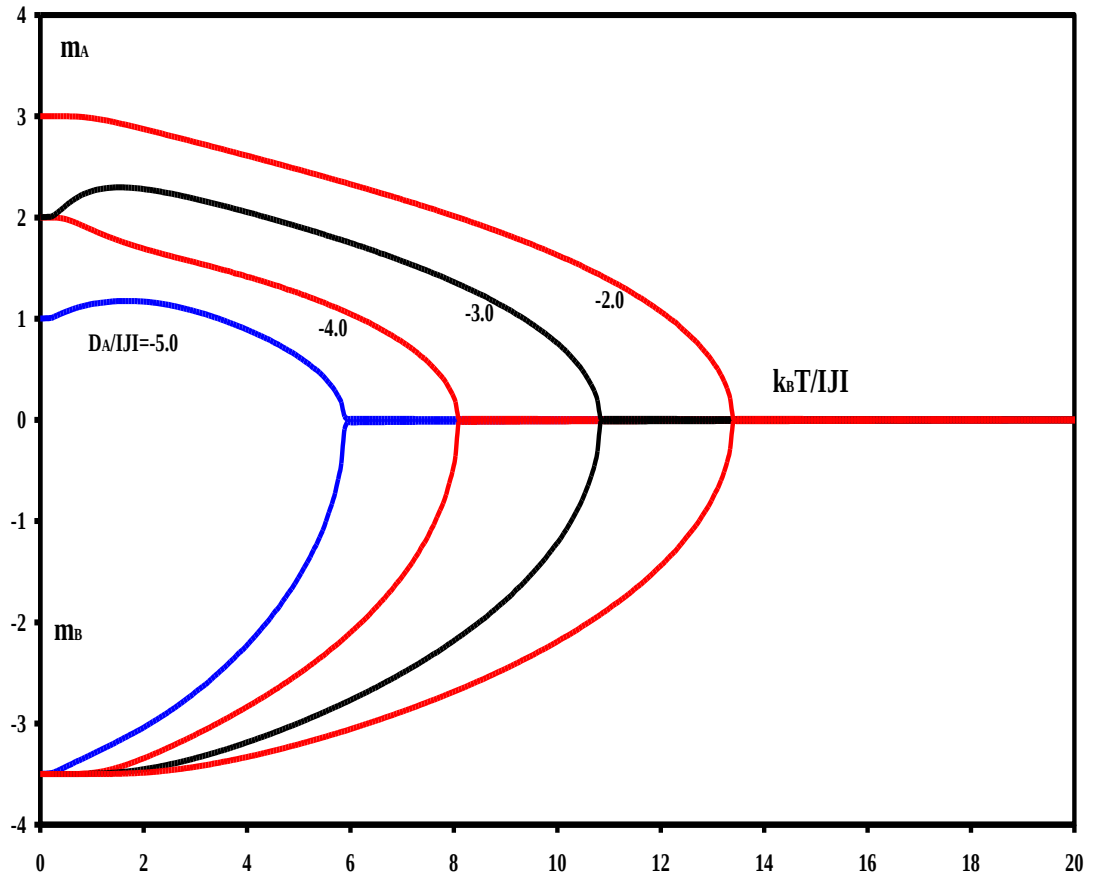
4.3 Magnetic Properties

4.3.1 Temperature Dependence of Sublattice and Total Magnetization

4.3.1a Square Lattice Structure ($z=4$)

Firstly, let us examine Fig.(4.3) stands for the sublattices magnetizations m_A, m_B for the mixed ferrimagnet ($z=4$), versus the absolute temperature for different values of

$D_A/|J|$, i.e., $-5.0 \leq D_A/|J| \leq -2.0$, with a fixed one of $D_B/|J| = -0.5$.



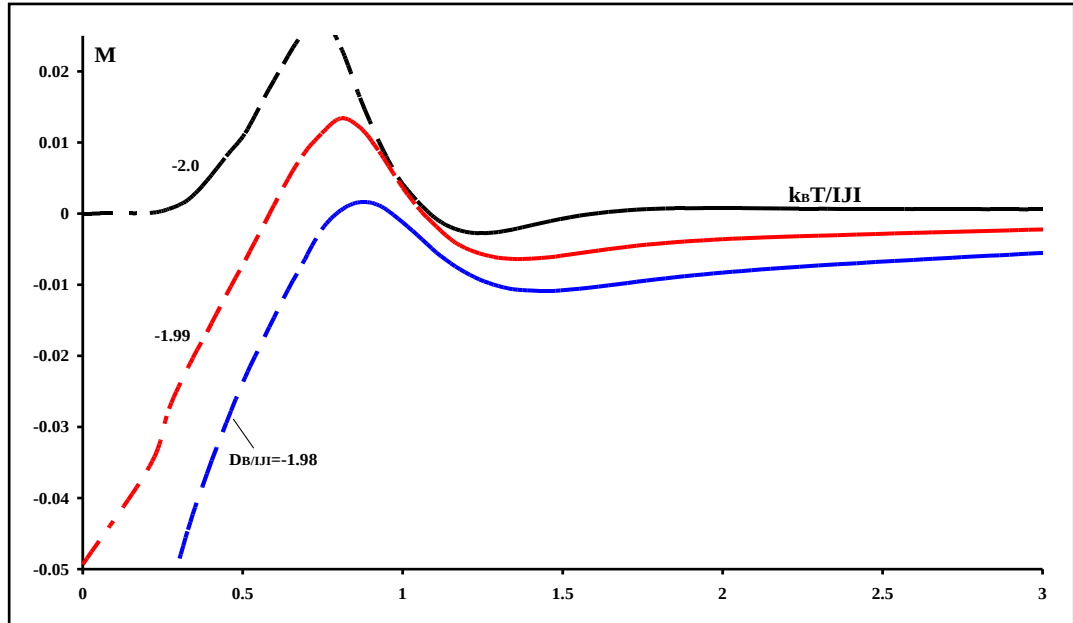
Figure(4.3). Temperature dependences of the sublattices magnetizations m_A, m_B for the mixed ferrimagnet

($z=4$), when the value of $D_A/|J|$ is changed, for fixed $D_B/|J| = -0.5$. The curves with values of

$D_A/|J| = -2.0, -3.0, -4.0, -5.0$ indicate characteristic behaviors at low temperature.

For Figures.(4.4), the sublattice magnetization m_A gives characteristic thermal variation behavior. However, as $D_B/|J|$ decreases from $D_B/|J| = -1.98$ for a fixed

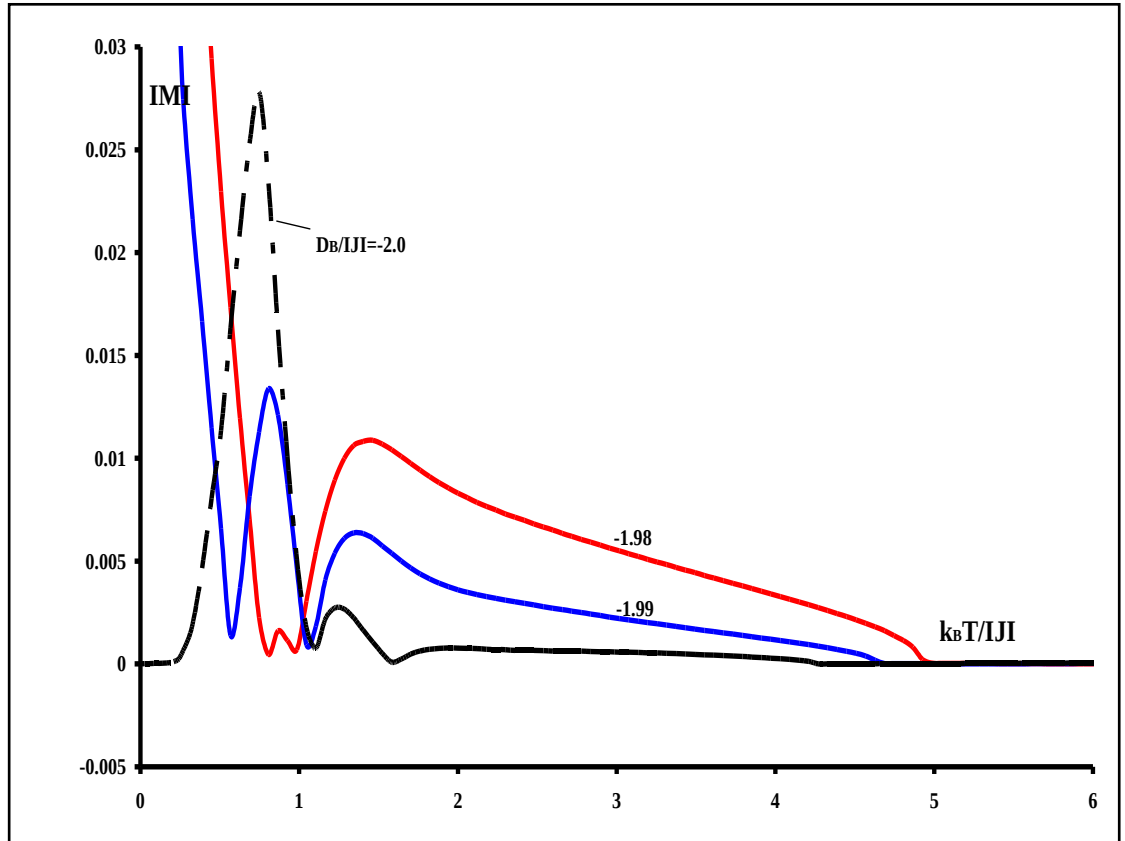
value of $D_A/|J|$, the temperature dependence of the total magnetization may exhibit interesting features as illustrated in Figs.(4.4),(4.5), respectively. The compensation temperature of a mixed spin-3 and spin-7/2 Blume-Capel ferrimagnet for square and simple cubic lattices is investigated in this correspondence. Let us now examine the magnetic properties(i.e., magnetic compensation and transition temperatures) of a ferrimagnet with characteristic crystal fields through which one can find distinguishable magnetic features for the proposed system. Fig.(4.4) displays the total magnetization versus the absolute temperature for different values of $D_B/|J|$. It is interesting to examine the characteristic properties of the system that we find the compensation temperature (T_k) depends strongly on the values of crystal fields $D_A/|J|$, and $D_B/|J|$ acting on the binary models suggested in the compounds $\text{Gd}_2\text{O}_2\text{S:Ln}^{3+}$ (Ln = Eu, Tb)[38,55]. As observed in Fig.(4.4), the system may have three compensation points at $k_B T/|J| = 0$ and $k_B T/|J| \neq 0$, respectively.



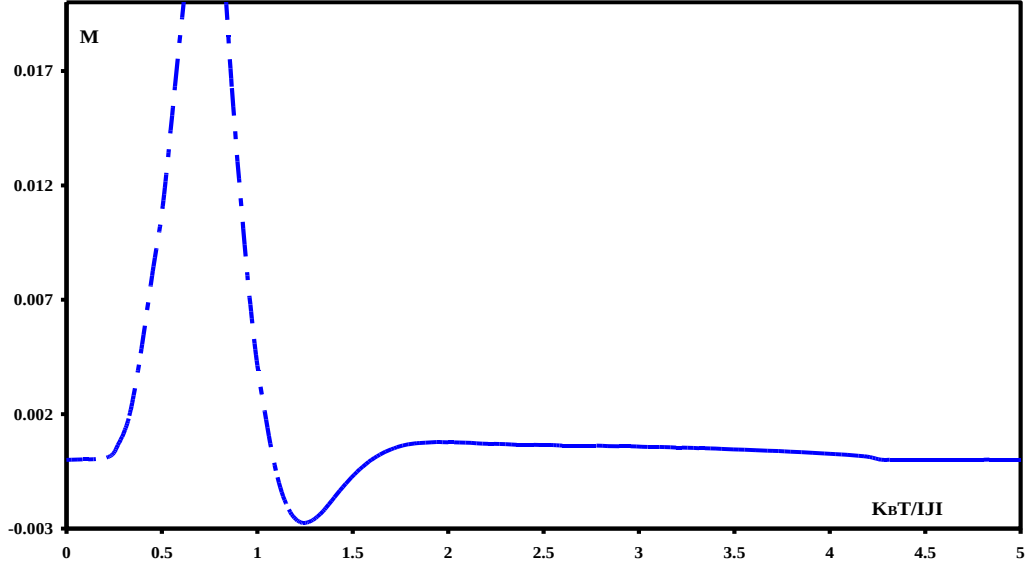
Figure(4.4). Temperature dependences of the total magnetization M for the mixed ferrimagnet ($z=4$),

when the value of $D_B/|J|$ is changed, for fixed $D_A/|J| = -1.985$.

Then, there is a response of the system for induction of three compensation temperatures in the range of negative values of magnetic crystal field, i.e., $-2.0 \leq D_B/|J| \leq -1.98$, with a fixed value of $D_A/|J| = -1.985$, acting on the A-atoms. Moreover, one can observe in the Fig.(4.5), the thermal variation dependence of the absolute magnetization value $|M|$ for the crystal lattice($z=4$) that may exhibit multicompensation points which can be obtained by solving the coupled equations for m_A and m_B numerically, depending on the values of the crystal fields, i.e., magnetic anisotropies(one can observe Eqs.(3.20),(3.21),and (3.28). It is clear, for the system, one may show the occurrence of compensation temperatures as in Refs[67,68].

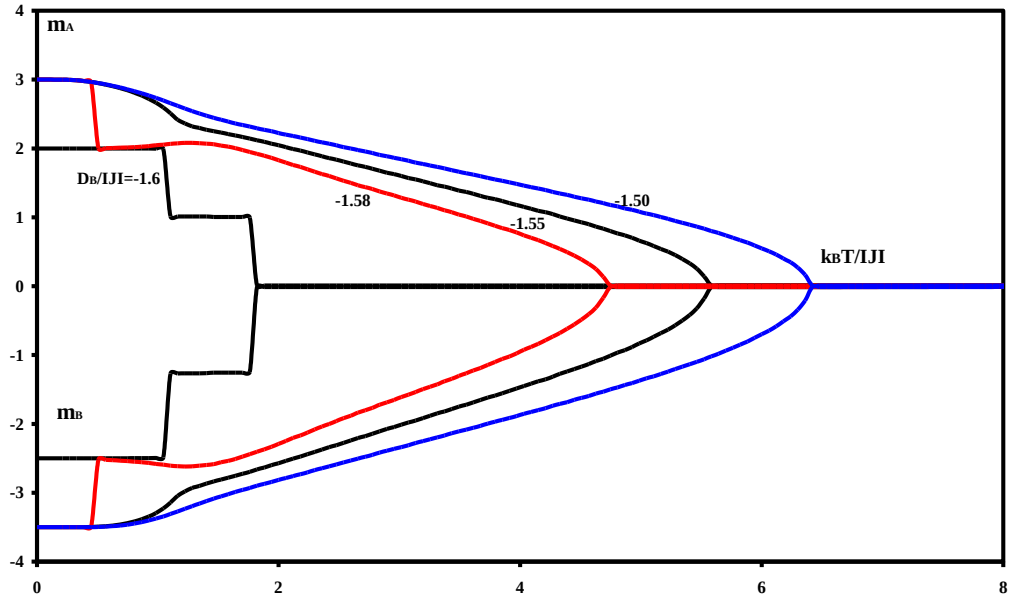


Figure(4.5). Temperature dependences of the absolute magnetization value $|M|$ for the mixed ferrimagnet ($z=4$), when the value of $D_B/|J|$ is changed, for fixed $D_A/|J| = -1.985$.



Figure(4.6). A close view of the temperature dependences of the total magnetization M for the mixed-spin Ising ferrimagnet with the coordination number $z=4$, when the values of $D_A/|J| = -1.985$, and

$$D_B/|J| = -2.0$$



Figure(4.7). Temperature dependences of the sublattices magnetizations m_A, m_B for the mixed ferrimagnet ($z = 4$), when the value of $D_B/|J|$ is changed, for fixed $D_A/|J| = -2.5$. The curves with values of $D_B/|J| = -1.50, -1.55, -1.58, -1.60$ indicate characteristic behaviors at low temperature.

Fig.(4.7) shows that a rather rapid decrease from its saturation magnetization occurs. Besides, the system is jumped at certain temperatures before being approached Curie

point. That is to say, for $T = 0$ $K^0, T > 0 K^o$, the system is passed through a second-order phase transition and then it moves to a first-order phase one in the range $-1.60 \leq D_B/|J| \leq -1.50$, namely, when $D_B/|J| = -1.58, -1.60$, for fixed $D_A/|J| = -2.5$. One can compare our results with those ones were obtained by H. Bouda et al[38], who have investigated mixed-spin systems having $S_i^A = 7/2$, $S_j^B = 3$, within the Monte-Carlo simulation.

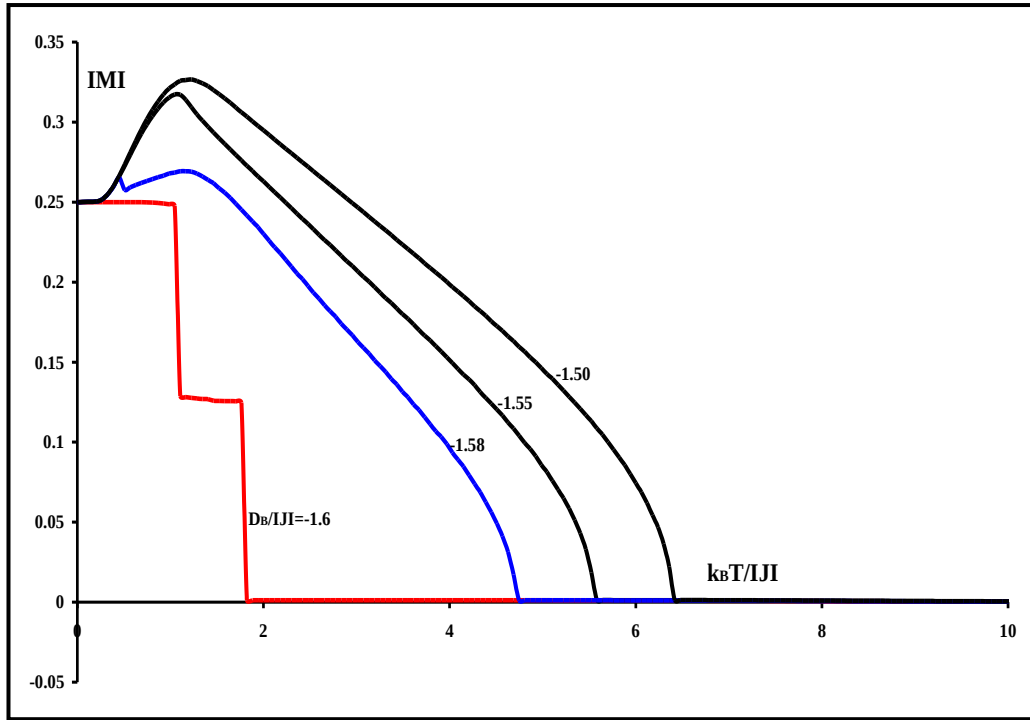
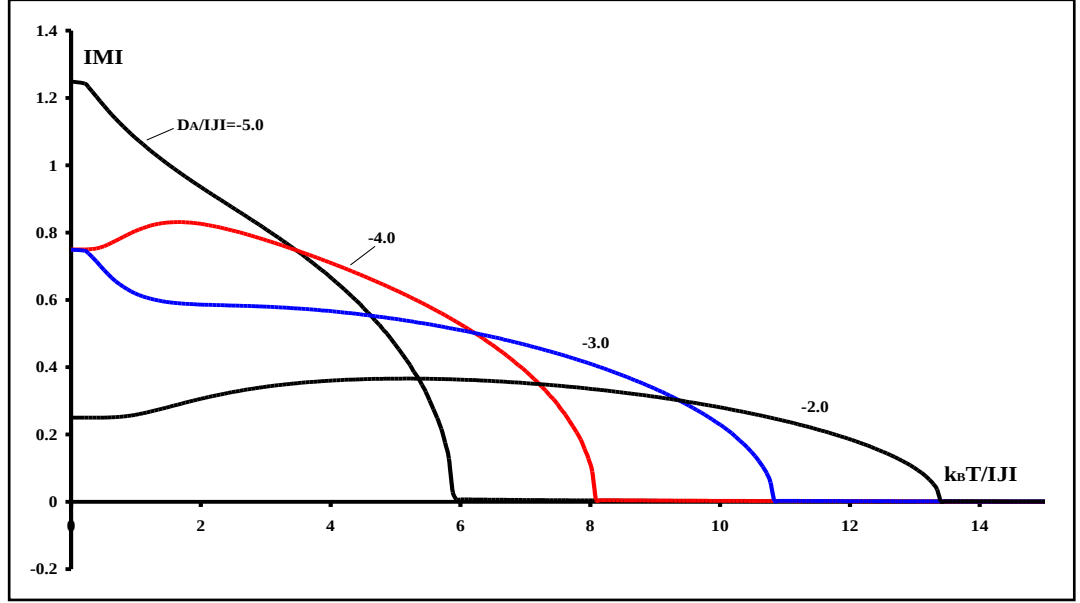


Figure (4.8). Temperature dependences of the absolute magnetization value $|M|$ for the mixed ferrimagnet ($z = 4$), when the value of $D_B/|J|$ is changed, for fixed $D_A/|J| = -2.5$.



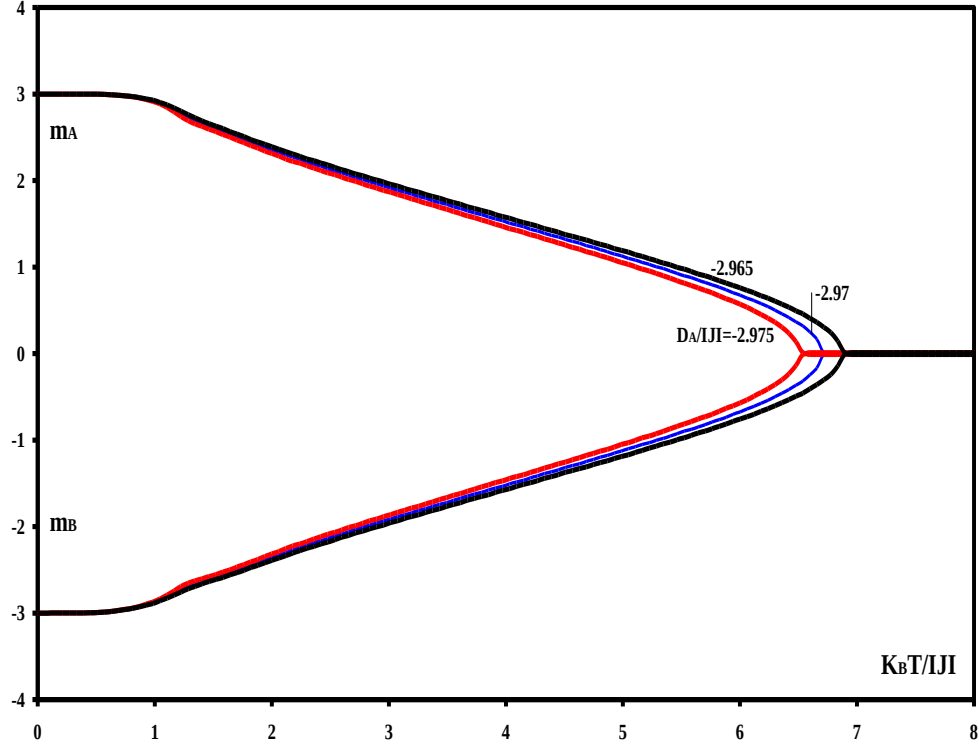
Figure(4.9). Temperature dependences of the absolute magnetization value $|M|$ for the mixed ferrimagnet ($z=4$), when the value of $D_A/|J|$ is changed, for fixed $D_B/|J| = -0.5$.

However, in Fig.(4.8), we report the thermal variations of the absolute magnetization value $|M|$ for the mixed ferrimagnet for a square lattice, when $D_B/|J| = -1.50, -1.55, -1.58, -1.60$, for fixed $D_A/|J| = -2.5$, respectively. Fig.(4.9) displays the thermal variations of the absolute magnetization value $|M|$ for the mixed ferrimagnet, when the value of $D_A/|J|$ is changed, for fixed $D_B/|J| = -0.5$. One can see an interesting feature of critical temperatures for selective values of crystal fields, i.e., magnetic anisotropies, in the range $-5.0 \leq D_A/|J| \leq -2.0$.

4.3.1b Simple cubic lattice Structure ($z = 6$)

On the other hand, we have interested in studying the magnetic compensation phenomenon of the mixed spin-3 and spin-7/2 ferrimagnetic system for a simple cubic lattice($z=6$). It is important to note the critical temperature depends not only on

the magnitudes of spin crystal fields but also on the structural lattice, one can see Figs.(4.10),(4.12),(4.13) and compare transition points with those ones as shown in Fig.(4.3), and Fig.(4.7), respectively[58-61].



Figure(4.10). Temperature dependences of the sublattices magnetizations for the mixed ferrimagnet

($z=6$), when the value of $D_A / |J|$ is changed, for fixed $D_B / |J| = -3.0$.

Notice that the sublattices magnetizations of the ordered phases that one can see Fig.(4.10), at $T > 0K$, are $m_A = 3$ and $m_B = -3$, which indicate in the ground state the spin configuration of S_j^B in the system consists of the mixed state; half of the spins on sublattice B are equal to $7/2$ and the other half of the spins on sublattice A are equal to 3 . It is worth to mention that the system may exhibit even three compensation points in certain anisotropy ranges of the magnetic atoms on two sublattices. The sublattice magnetization undergoes to cancel but it is still incomplete so there is

spontaneous magnetization of the remaining in the system(i.e., $M \neq 0$), this is evidence to the antiferromagnetic near neighbor interactions.

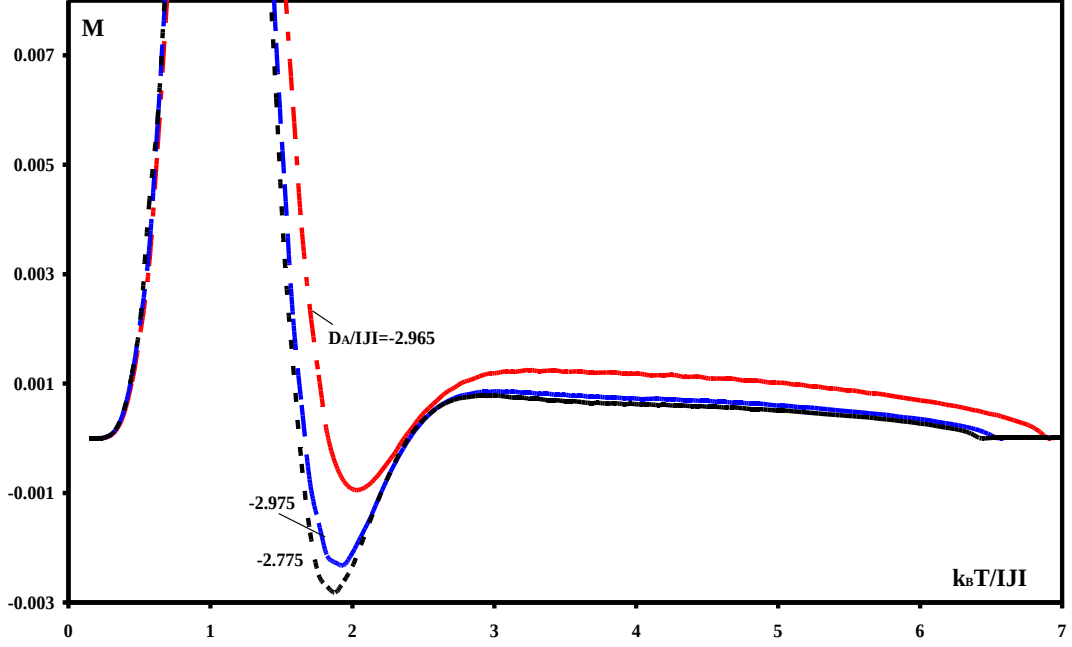


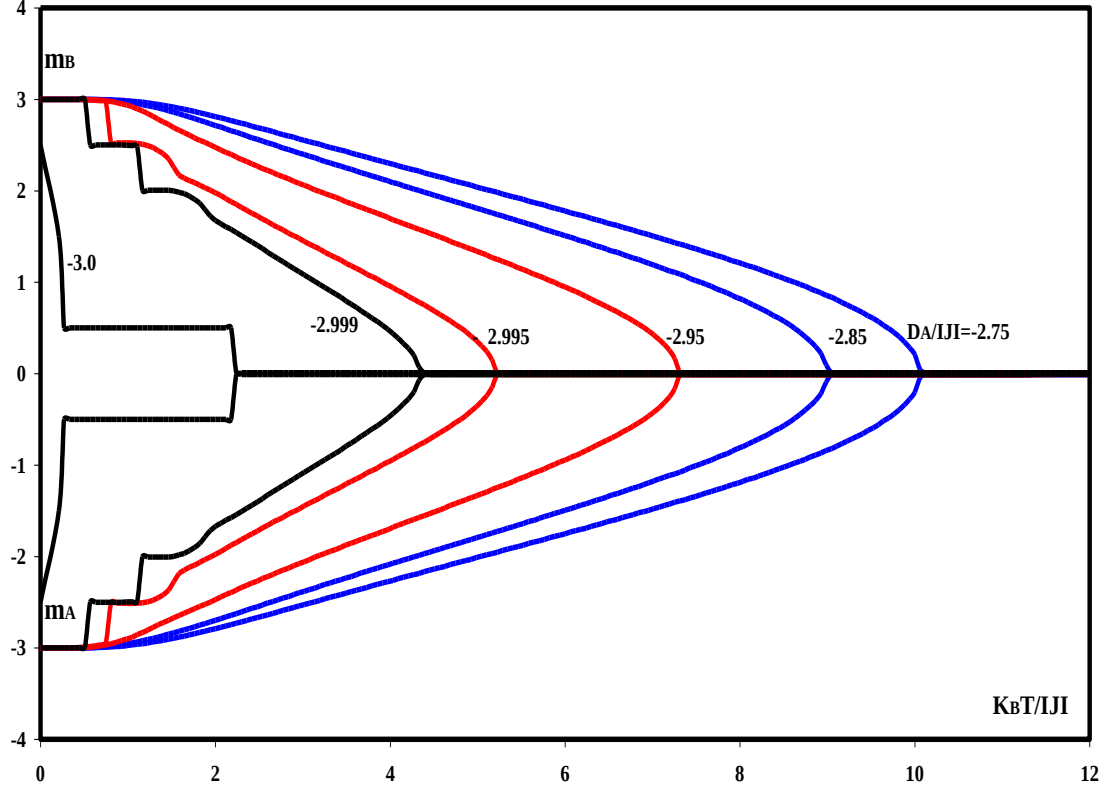
Figure (4.11). Temperature dependences of the total magnetization M for the mixed ferrimagnet ($z=6$), when the value of $D_A/|J|$ is changed, for fixed $D_B/|J| = -3.0$.

$$z=6), \text{ when the value of } D_A/|J| \text{ is changed, for fixed } D_B/|J| = -3.0.$$

This interaction tends to align the spins adjacent in opposite directions as the rising temperature of the system, and therefore the direction of this residual magnetization can switch because of the thermal excitation. The compensation behaviors shown in Figs.(4.4),(4.5),(4.11), indicate the crossing points between the magnitudes of m_A and m_B which prove the eligibility of Eqs.(3.21) and (3.21), respectively. On the other hand, we report that the proposed model is jumped at certain temperatures before being reached the transition temperature T_C . Figs.(4.12),(4.13) stand for the thermal variations of the sublattices magnetizations for the mixed ferrimagnet($z=6$), indicating characteristic behaviors at low temperature. However from Fig.(4.12) system is passed through a second-order

phase transition and then it moves to a first-order when

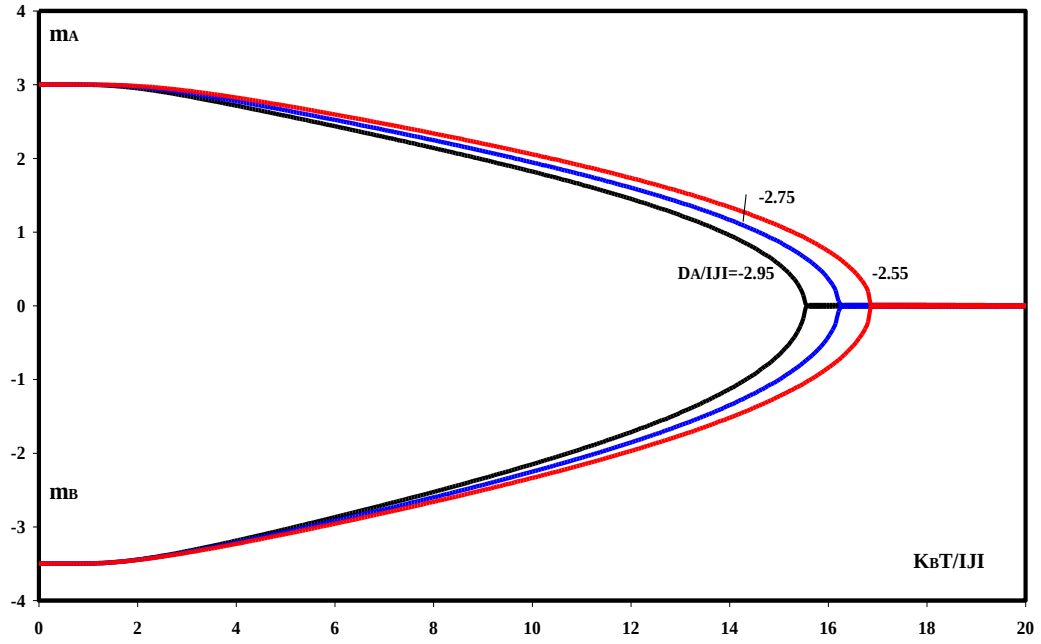
$D_A/|J| = -2.75, -2.85, -2.85, -2.95, -2.995, -2.999, -3.0$, for fixed $D_B/|J| = -3.0$.



Figure(4.12). Temperature dependences of the sublattices magnetizations m_A, m_B for the mixed ferrimagnet($z=6$), when the value of $D_A/|J|$ is changed, for fixed $D_B/|J| = -3.0$. The curves

with values of $D_A/|J| = -2.75, -2.85, -2.85, -2.95, -2.995, -2.999, -3.0$, indicate

characteristic behaviors at low temperature.



Figure(4.13). Temperature dependences of the sublattices magnetizations m_A, m_B for the mixed ferrimagnet ($z=6$), when the value of $D_A / |J|$ is changed, for fixed $D_B / |J| = -2.0$.

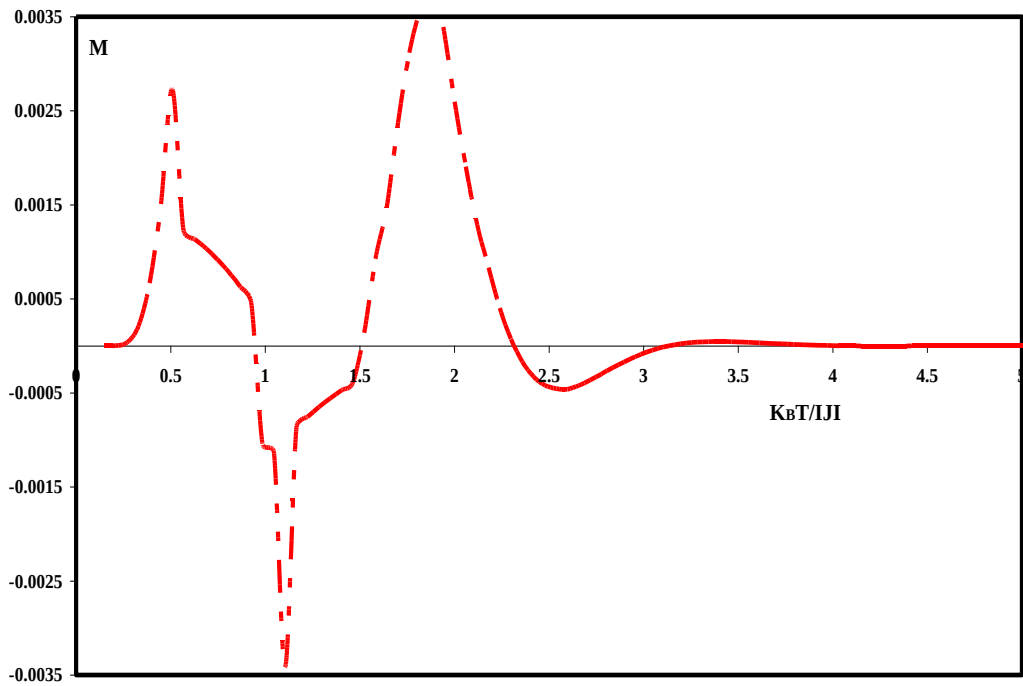
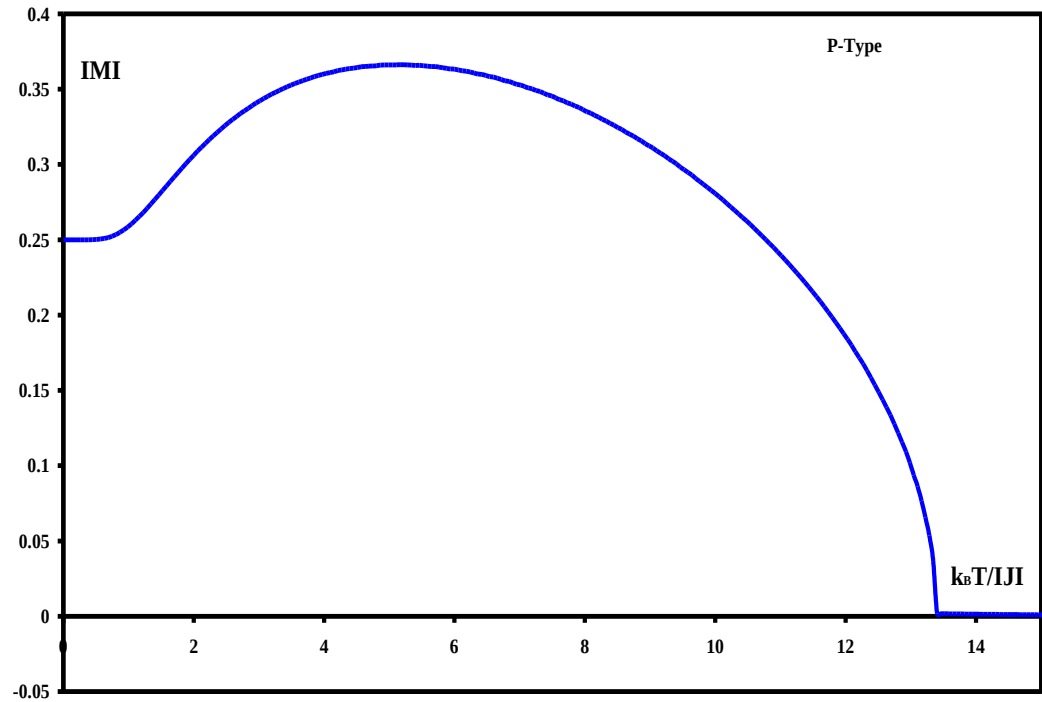


Figure.14. A close view of the temperature dependences of the total magnetization M for the mixed–spin Ising ferrimagnet with the coordination number $z=6$, when the values of $D_A / |J| = -2.999$, and

$$D_B / |J| = -3.0.$$

4.3.2 Types of Ferromagnetic Behaviors

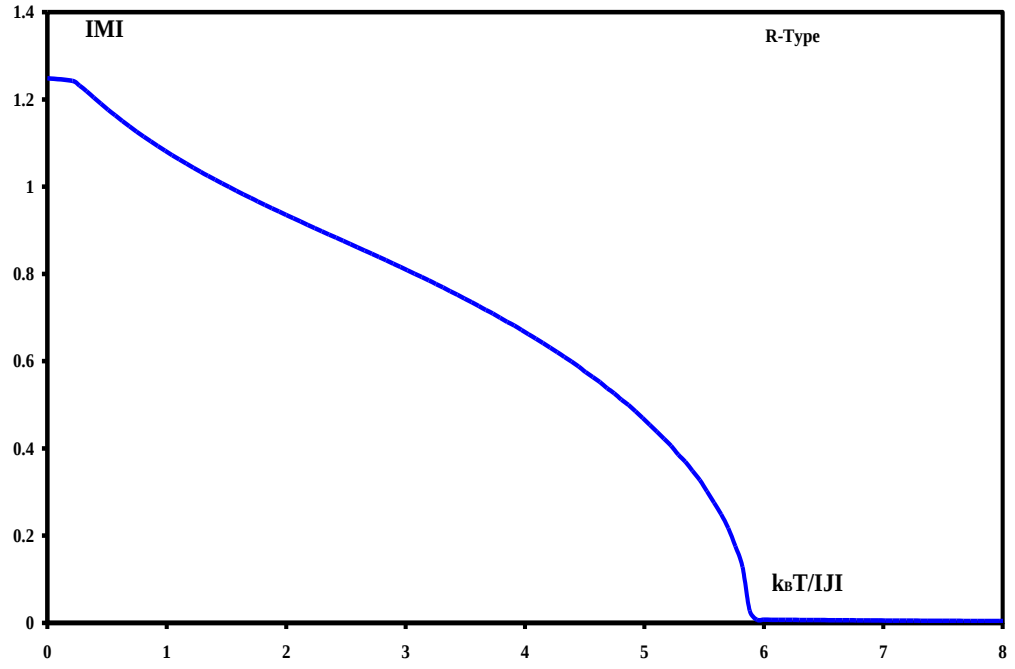
Besides, the model undergoes three types with different behaviors which are R-, P-, and S-type, respectively. These results can be compared to those of Monte Carlo simulation within the Metropolis algorithm; the Hamiltonian of the system includes the interaction between the first nearest neighbors and the crystal fields generated by the spin-7/2 and spin-3[38]. However, the authors of Ref.[38] focused into the effect of a positive single-ion anisotropy on the phase diagrams of a system considered with crystal fields acting only on spin-3 atoms. Now, we examine the total magnetization with thermal variations and acquired compensation types of the Ising model. Figures((4.15)-(4.20)), illustrate the thermal dependence of total magnetization $|M|$ for certain values of magnetic anisotropies. One can observe those figures that the considered model undergoes six types of different behaviors which are L-, M-, P-, R-, S-, and W-type of magnetic behaviors observed in the proposed system, one can see Figs.((4.15), (4.16), (4.17), (4.18), (4.19), and (4.20)), respectively. This is a good agreement with those types predicted in Ref [69]. The presence of spin compensation points has been shown to be dependent of negative magnetocrystalline fields, namely, $D_A|J| \leq -1.98$; however, the magnitudes of these points in the temperature space are affected, for the square mixed ferrimagnet ($z=4$), and simple cubic mixed one ($z=6$), respectively.



Figure(4.15). Temperature dependences of the absolute magnetization value $|M|$ for the mixed

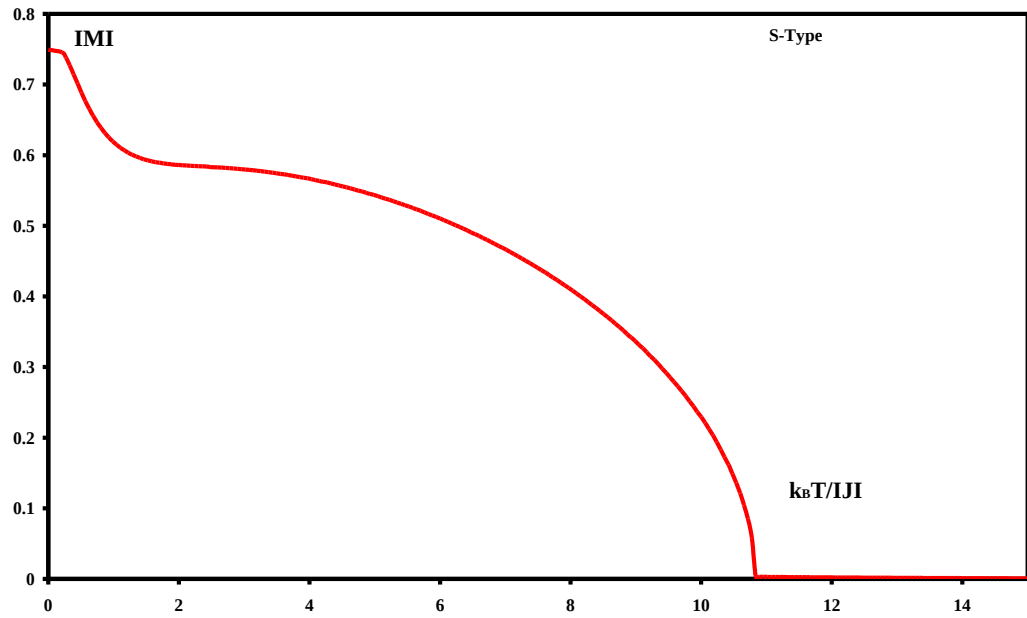
ferrimagnet ($z=4$), when the values of $D_A/|J| = -2.0$, and $D_B/|J| = -0.5$

The appearance of these curves is strongly dependent on the negative crystal fields domains. Finally, let us confirm the temperature dependence of the total magnetization depending on the values of anisotropies, i.e., crystal fields $D_A/|J|$ of the sites occupied by atoms-A for a specific value of $D_B/|J| = -3.0$. As shown in Fig.(4.14), the system may exhibit characteristic features that, it is possible to have many compensation points at $T \neq 0K^\circ$, namely, for a simple cubic lattice.



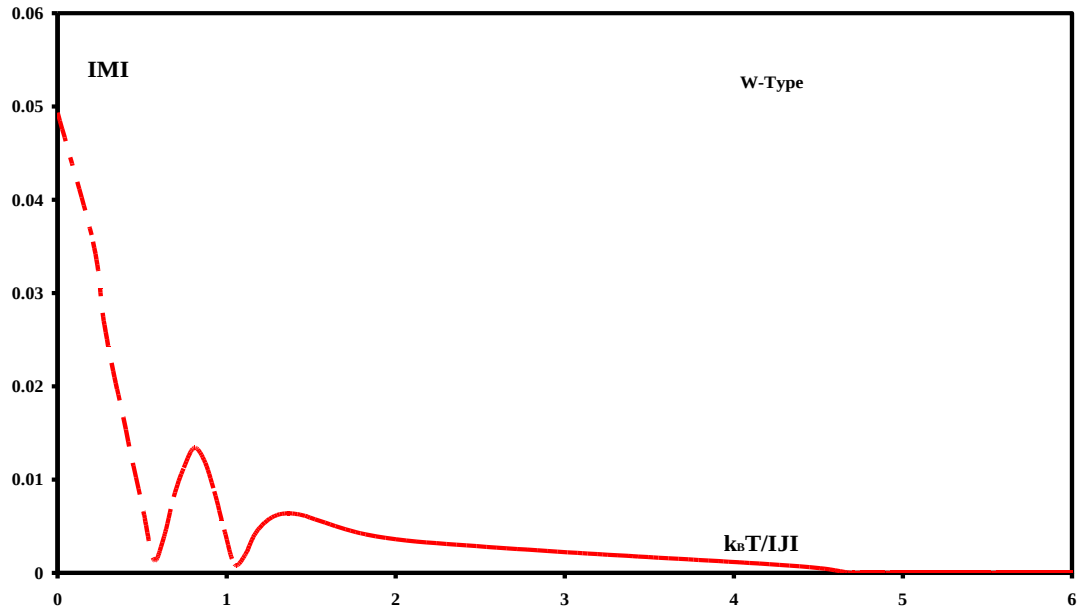
Figure(4.16). Temperature dependences of the absolute magnetization value $|M|$ for the mixed

ferrimagnet ($z=4$), when the values of $D_A/|J| = -5.0$, and $D_B/|J| = -0.5$.

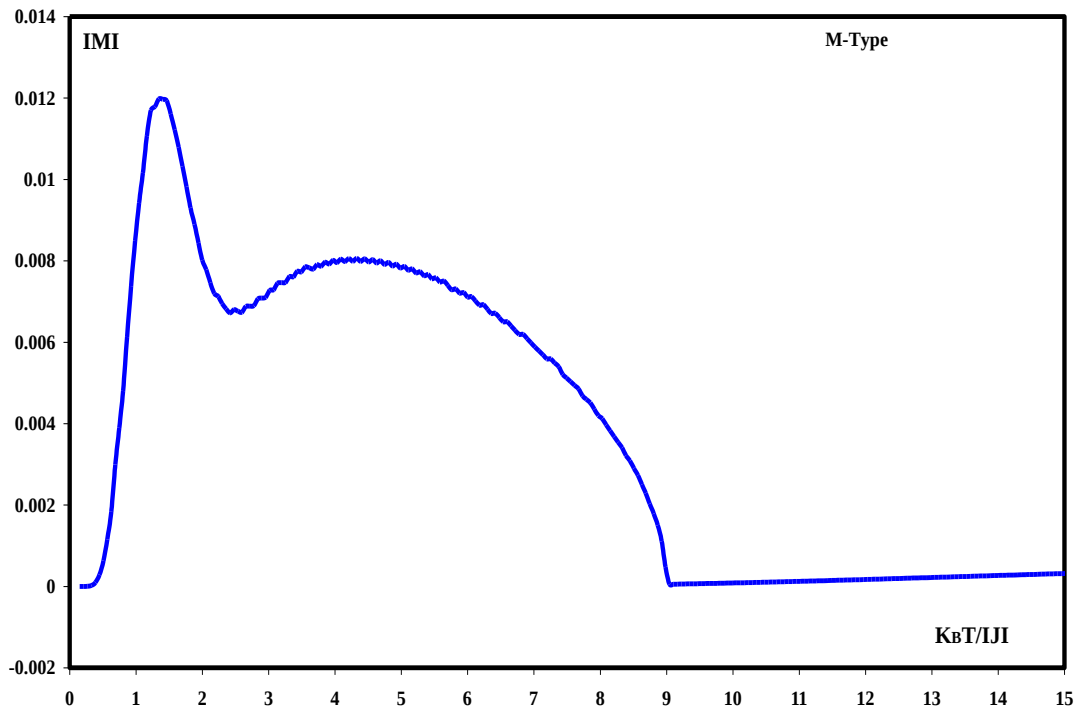


Figure(4.17). Temperature dependences of the absolute magnetization value $|M|$ for the mixed

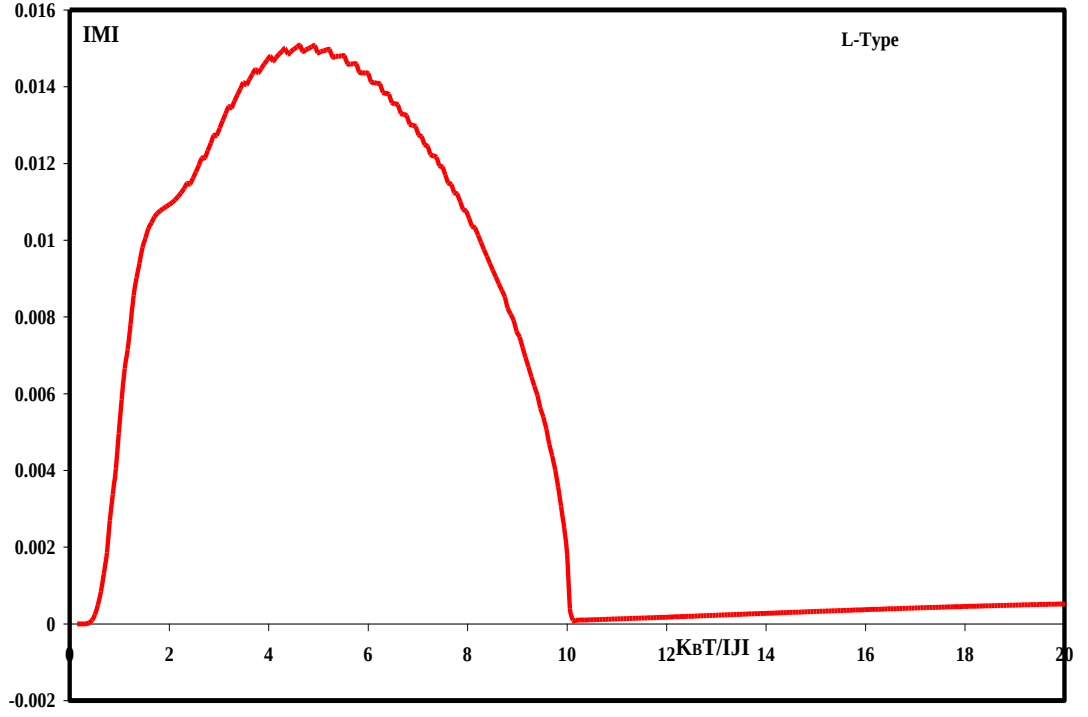
ferrimagnet ($z=4$), when the values of $D_A/|J| = -3.0$, and $D_B/|J| = -0.5$.



Figure(4.18). Temperature dependences of the absolute magnetization value $|M|$ for the mixed ferrimagnet ($z=4$), when the values of $D_A / |J| = -1.985$, and $D_B / |J| = -1.99$.



Figure(4.19). Temperature dependences of the absolute magnetization value $|M|$ for the mixed ferrimagnet ($z=6$), when the values of $D_A / |J| = -2.85$, and $D_B / |J| = -3.0$.



Figure(4.20). Temperature dependences of the absolute magnetization value $|M|$ for the mixed

ferrimagnet ($z=6$), when the values of $D_A/|J| = -2.75$, and $D_B/|J| = -3.0$

4.3.3 Crystal Field Dependence of Transition Temperature

In this section, it is interesting to investigate the magnetic properties(i.e., the phase diagrams) of the system that we find the transition(or critical) temperature depends strongly on the values of crystal fields D_A, D_B acting on the A – and B – atoms, respectively. Fig.(4.21) shows high-temperature phase diagram in the $(D_B/|J|, K_B T_C/|J|)$ plane for a square lattice($z=4$), where the transition temperature can be determined by requiring that the sublattice magnetization m_A, m_B tend to zero continuously as the temperature is closed to Curie point.

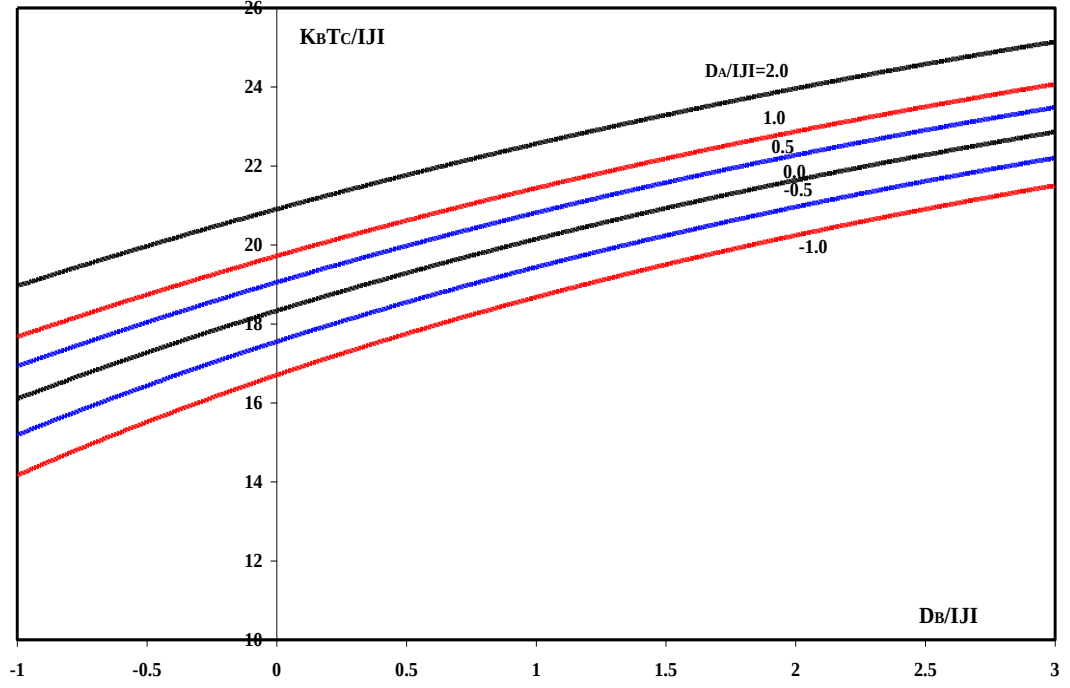


Figure.(4.21): Phase diagram in the $(D_B/|J|, K_B T_C/|J|)$ plane for the mixed-spin Ising ferrimagnet with the coordination number $z=4$, when the value of D_A is changed. The solid lines indicate second-order phase transitions.

It has been observed, for both figures(Figs.(4.20),(4.21)), that the ordered states exist at high temperatures for all values of crystal fields. So, one can obtain a transition temperature($k_B T/|J| = 18.25$, and $k_B T/|J| = 18.328$, for Figs.(4.21), (4.22), respectively, i.e., particularly, in the absence of anisotropies, i.e., magnetic crystal fields($D_A = D_B = 0.0$). Moreover, one can see from Fig.(4.22), at the values of $D_B/|J| \geq 1.0$, the transition temperature can never be increased[59]. Fig(4.23) shows the phase diagrams in the $(D_B/|J|, K_B T_C/|J|)$ plane for various values of $D_A/|J|$, on a simple cubic lattice. We see that a certain type of phase diagram is achieved with second-order transitions at different values of transition temperature.

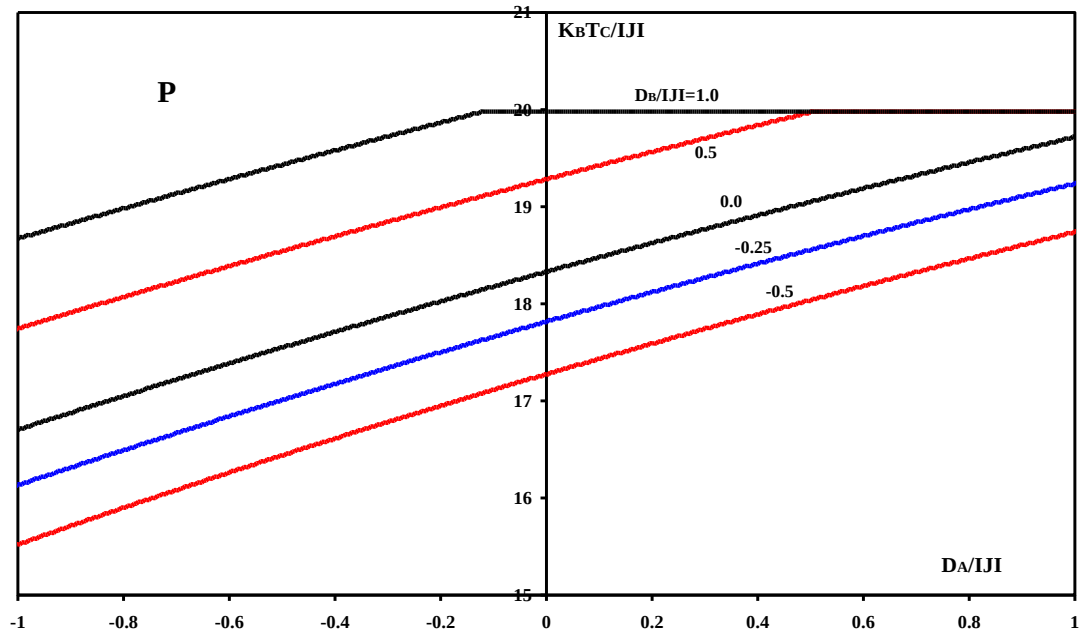


Figure.(4.22): Phase diagram in the $(D_A/|J|, K_B T_C/|J|)$ plane for the mixed-spin Ising ferrimagnet with the coordination number $z=4$, when the value of D_B is changed. The solid lines indicate second-order phase transitions. P is the paramagnetic state.

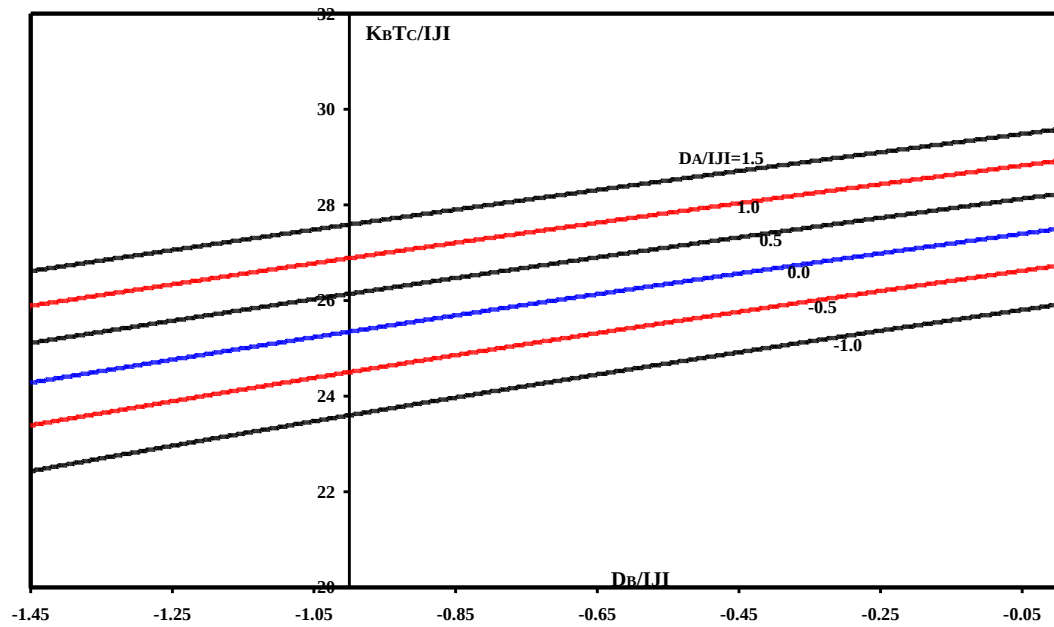


Figure.(4.23): Phase diagram in the $(D_B/|J|, K_B T_C/|J|)$ plane for the mixed-spin Ising ferrimagnet with the coordination number $z=6$, when the value of D_A is changed. The solid lines indicate second-order phase transitions.

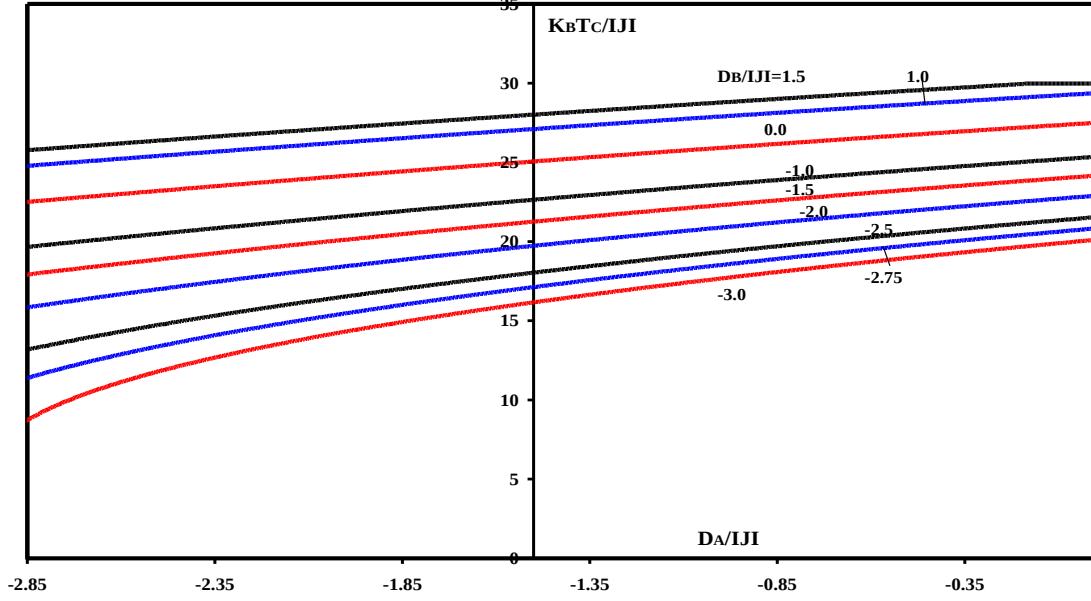


Fig.(4.24): Phase diagram in the $(D_A/|J|, K_B T_C/|J|)$ plane for the mixed-spin Ising ferrimagnet with the coordination number $z=6$, when the value of D_B is changed. The solid lines indicate second-order phase transitions.

It has been observed, for both figures(Figs.(4.21),(4.23)), that the ordered states exist at high temperatures for all values of crystal fields. So, one can obtain transition temperatures, $k_B T_C/|J| = 18.25$, and $k_B T_C/|J| = 18.328$, for Figs.(4.21), (4.23), respectively, i.e., particularly, in the absence of anisotropies, i.e., magnetic crystal fields($D_A = D_B = 0.0$). Moreover, one can see from Fig.(4.23), at the values of $D_B/|J| \geq 1.0$, the transition temperature can never be increased[59]. On the other hand, as noted above(i.e., one can observe Fig.(4.22)), it has been investigated the second order phase transitions lines in the range $-0.5 \leq D_A/|J| \leq 2.5$. Fig(4.23) shows the phase diagrams in the $(D_B/|J|, K_B T_C/|J|)$ plane for various values of $D_A/|J|$, on a simple cubic lattice. Whereas, in Fig.(4.24), one finds a characteristic behavior at the values of $D_B/|J| \geq 1.5$, that the transition temperature can never be increased. We see that a considered type of phase diagram is achieved with second-

order transitions at different values of transition temperature. That is to say, phase transitions related to anisotropy continuity showing second-order behavior. It is worthwhile to note that the second-order phase transition lines are analytically obtained through a Landau free energy expansion in the order parameter, that one is able to evaluate equation(3.27), by setting $a = 0$ [59,70].

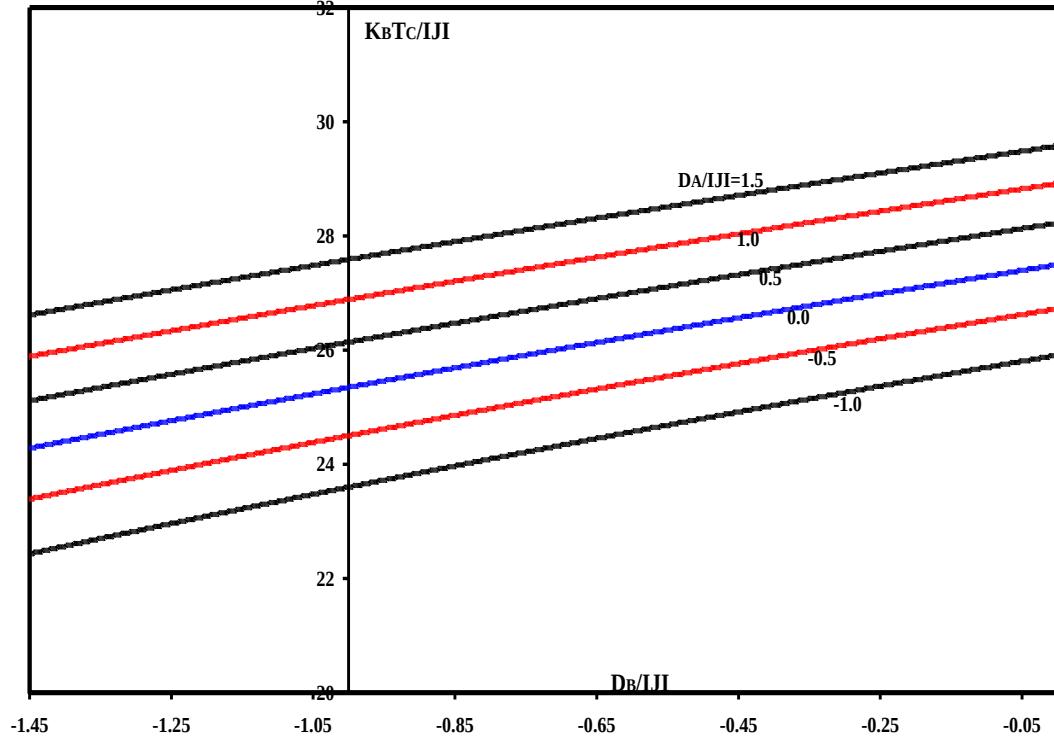


Fig.(4.25): Phase diagram in the $(D_B/|J|, K_B T_C/|J|)$ plane for the mixed-spin Ising ferrimagnet with the coordination number $z=6$, when the value of D_A is changed. The solid lines indicate second-order phase transitions.

Besides, one can compare the results of transition temperatures(Fig.(4.12)) with those one obtained in Figs.(4.25), (4.26), respectively. However, for a simple cubic lattice, in the range $-2.75 \leq D_B/|J| \leq 1.5$, or a square lattice in $-2.0 \leq D_B/|J| \leq 2.5$, it is observed Fig.(4.27), and Fig.(28), respectively). In the figures, we show, for different values of D_B , the phase diagrams in the (D_A, T) plane of the mixed-spin

Blume-Capel Ising ferrimagnet, that one can see, for both cases, there is long-range order for the regions have been investigated[68].

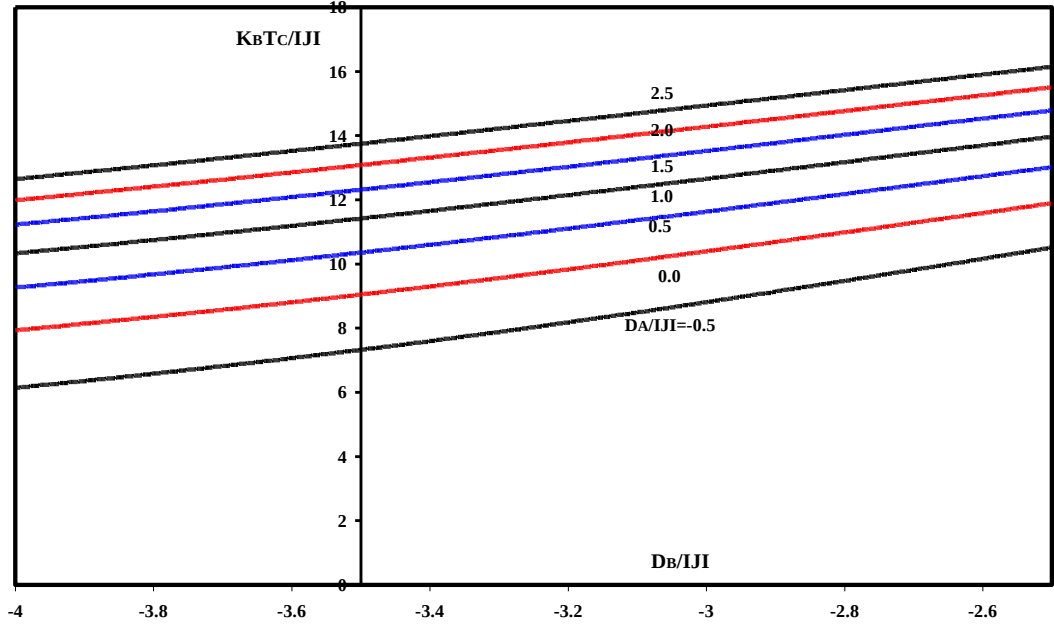


Fig.(4.26): Phase diagram in the $(D_B/|J|, K_B T_C/|J|)$ plane for the mixed-spin Ising ferrimagnet with the coordination number $z=4$, when the value of D_A is changed. The solid lines indicate second-order phase transitions.

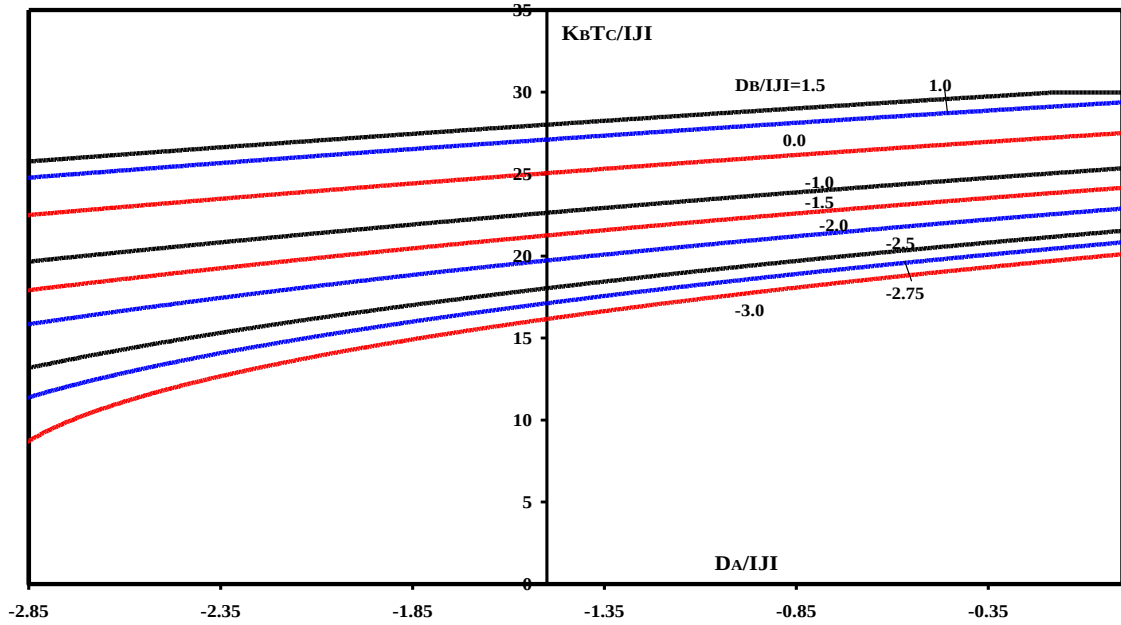


Fig.(4.27): Phase diagram in the $(D_A/|J|, K_B T_C/|J|)$ plane for the mixed-spin Ising ferrimagnet with the coordination number $z=6$, when the value of D_B is changed. The solid lines indicate second-order phase transitions.

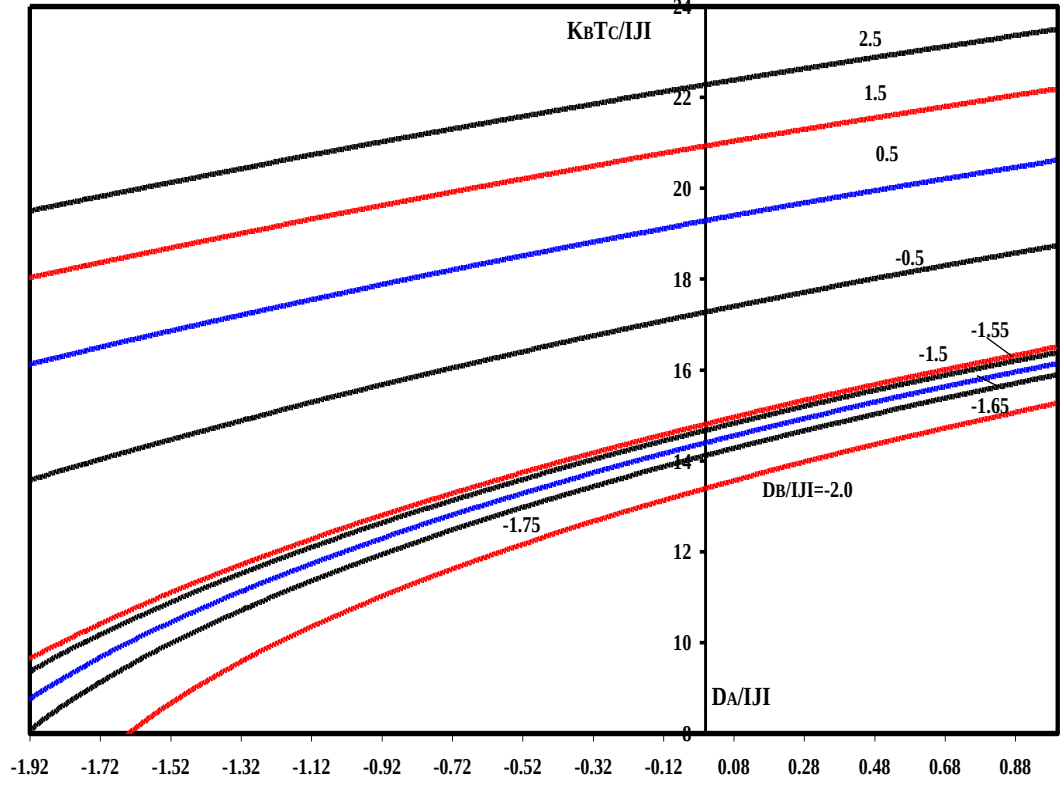


Figure.(4.28): Phase diagram in the $(D_A/|J|, K_B T_C/|J|)$ plane for the mixed-spin Ising ferrimagnet with the coordination number $z=4$, when the value of D_B is changed. The solid lines indicate second-order phase transitions.

On the other hand, for a simple cubic lattice, in the range $-2.75 \leq D_B/|J| \leq 1.5$, or a square lattice in $-2.0 \leq D_B/|J| \leq 2.5$, one can see Figure.(4.27), and Figure.(28), respectively). In the figures, we show, for different values of D_B , the phase diagrams in the (D_A, T) plane of the mixed-spin Blume-Capel Ising ferrimagnet, that one can see, for both cases, there is long-range order for the regions have been investigated[68].

Chapter Five

Conclusions and Future Works

5.1 Conclusions

Within reviewing the results of the ferrimagnetic mixed spin-3 and spin-7/2 Blume-Capel Ising system using mean-field approximation (MFA), we can conclude that:

1. For a square lattice($z=4$) there is a response of the system for induction of three compensation temperatures in the range of negative values of magnetic crystal field, i.e., $-2.0 \leq D_B/|J| \leq -1.98$, with a fixed value of $D_A/|J| = -1.985$, acting on the A- atoms.
2. The proposed system has many compensation temperatures in the range of $-2.999 \leq D_A/|J| \leq -2.55$ with fixed values of $D_B/|J| = -2.0$, and $D_B/|J| = -3.0$, respectively, for a simple cubic lattice ($z=6$).
3. The proposed system undergoes the first and second order phase transitions; however, the second order phase transition is the dominant in revealing the properties of the system in the planes $(m_A, K_B T/|J|), (m_B, K_B T/|J|)$, as shown in Figs.((4.3), (4.7), (4.10),(4.12)). It is worth to mention that one can recognize among these phases which appear in our system within studying the behaviors in the space of $(D_A/|J|, K_B T_C/|J|)$ as depicted in Figures.((4.21), (4.22), (4.23),(4.24)), respectively.
4. We have obtained new phases for the proposed system namely (3, -3), and (2.5,-2.5), for appropriate values of anisotropies, i.e., crystal fields $(D_A/|J| = -2.75, -2.85, -2.85, -2.95, -2.995, -2.999, -3.0)$, for fixed $D_B/|J| = -3.0$, as shown in Figs.(4.11),(4.12), respectively.
- 5- The system experiences a jump which corresponds to the first – order transition to obtain the phase is (2,-2.5) when $(D_A/|J| = -2.5)$, $(D_B/|J| = -1.6)$ and the new one is (2.5.-2.5) , for $(D_A/|J| = -3.0)$, as show in(fig.5),(fig.10) , respectively.

6- It has been reported that the present magnetic system undergoes six types of different behaviors which are L-, M -, P-, R- , S-, AND W – type, respectively.

7- Transition temperatures are effectively increased with increasing the magnetic anisotropy for sublattice of B-atoms in the range $-2.75 \leq D_B / |J| \leq 1.5$ with different values of $D_A / |J|$.

8. It is worth to note that our results concerning the number of compensation points are more better than the results obtained by Monte-Carlo (MC) (one can observe Ref.[39]),

5.2 Future Works

1. Studying second – order phase transitions for a mixed spin – 3 and spin -7/2 Blume-capel Ising ferrimagnet under influence of an external magnetic field.
2. Studying first - order phase transitions for a mixed spin -3 and spin 7/2 Blume – Caple Ising lattices: body-center cubic lattice , and face – centered cubic one.
3. Studying thermodynamic functions of the proposal system such as internal energy , ferrimagnetic susceptibility and the entropy .
4. Studying the magnetic hysteresis loops of a mixed spin – 3 and spin – 7 using Blume- Caple Ising model
5. Studying the thermal properties of a mixed spin -3 and spin – 7 Ising ferrimagnetic .

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List of Publication

1. Ali Arabi Abed, and Hadey K. Mohamad. "Magnetic characteristics of a mixed spin-3 and spin-7/2 Blume-Capel system for square and simple cubic lattices." *Solid State Communications* 338 (2021): 114456.
2. Ali A. Abed' and Hadey K. Mohamad. " Ferrimagnetic compensation temperatures in the mean-field theory of a mixed spin-3 and spin-7/2 Blume-Capel Ising Model.Al In 1st "International Conference on Advanced Research in Pure and Applied Science", AL Muthanna university , samawah , Iraq to be published in **AIP** conference proceeding 2021.

الخلاصة

في هذه الدراسة ، تمت دراسة التحولات الطورية المغناطيسية ضمن نطاق المغناط الجزيئية ، باستخدام طريقة متوسط المجال (MFMM). تجدر الإشارة إلى أنه تم تطبيق توزيع بلوم-كابيل (Blume-Capel Configuration (BCC على نظام فيرميغناطيسي خليط يتكون من شبكتين عزومها المغناطيسية (7/2 ، 3) . تم إنشاء مخطط طوري للحالة الأرضية لشبكة مربعة ولشبكة مكعب بسيط في المستوي ($D_A/|J|$, $D_B/|J|$) على التوالي. بموجب متباينة بوكوليوبوف (Bogoliubov inequality)(BI) للطاقة الحرة ، فقد تم في هذه الدراسة تحفيز ظاهرة التعادل البرمي والتنبؤ أيضًا بالنقاط الحرجة المميزة ، أي بمعنى إيجاد العديد من درجات الحرارة التعويضية المغناطيسية للنموذج المقترح. وقد حصلنا على نتائج جديدة للشبكة المكعبة مما يشجع العمل التجريبي في المركبات ($Gd_2O_2S: Ln_3 + (Ln = Eu, Tb)$ من ناحية أخرى ، تم نشر دالة الطاقة الحرة على أساس نظرية لاندau Landau Theory لحساب خطوط التحولات الطورية من الرتبة الثانية التي يمر بها النظام قيد البحث. ان دالة الطاقة الحرة وجدت كدالة للتمغنط الفرعية للشبائك البلورية المقترحة باستخدام دالة التقسيم القانونيه z ، عليه تم تغيير التباينات المغناطيسية للشبكتين الفرعيتين بدقة بحيث تمكنا من دراسة الظواهر المثيرة للاهتمام مثل سلوكيات التعادل المغناطيسي وكذلك انواع مميزة لدوال التمغنط الكلي وتمغنط الشبائك الفرعية وعلاقتها بدرجات الحرارة المطلقة للنظام. في هذه الدراسة وجد ان النظام المغناطيسي المقترح يمتلك نقاط تعادل متعددة عند مدى التباينات المغناطيسية للذرات $-2.55 \leq D_A/|J| \leq -2.999$ بثبوت $D_B/|J|$ عند القيم $D_B/|J| = -2.0$ و $D_B/|J| = -3.0$ ، إلى جانب ذلك ، تم الحصول على سلسلة من أنواع السلوكيات لشبكة مكعب بسيط وشبكة مربعة على التوالي، وهي L- و M- و P- و R- و S- و W. ويبقى أن نذكر أن حدوث درجة الحرارة التعويضية له أهمية كبيرة في تكنولوجيا الاتصالات لأنه في هذه الدرجة الحرارية بالذات نحتاج الى اقل مقدار ممكن من المجال المعاكس لتغيير اتجاه التمغنط عند اكمال حلقة الهسترة المغناطيسية وهكذا يمكن الحصول على حلقة هسترة ذات مساحة اقل .



وزارة التعليم العالي والبحث العلمي

جامعة المثنى كلية العلوم

قسم الفيزياء

دراسة التحولات الطورية من الرتبة الثانية لنظام فيريمغناطيسي خليط باستخدام نشر لاندאו

رسالة مقدمة الى مجلس كلية العلوم / جامعة المثنى كجزء من متطلبات نيل درجة الماجستير
في علوم الفيزياء

من قبل الطالب

علي عربي عبد جبر

بكالوريوس علوم فيزياء تطبيقية 2007

بإشراف

أ.م.د. هادي قاسم محمد