**DOKUZ EYLÜL UNIVERSITY**
**GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES**

# SPIN-S ISING MODEL IN A MAGNETIC FIELD: AN EFFECTIVE - FIELD THEORY ANALYSIS

**by**
**Yücel CANPOLAT**

**July, 2007**
**İZMİR**

# SPIN-S ISING MODEL IN A MAGNETIC FIELD:AN EFFECTIVE - FIELD THEORY ANALYSIS

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**Yücel CANPOLAT**

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We have read the thesis entitled **"SPIN-S ISING MODEL IN A MAGNETIC FIELD: AN EFFECTIVE-FIELD THEORY ANALYSIS "** completed by **YÜCEL CANPOLAT** under supervision of **PROF. DR. HAMZA POLAT** and we certify that in our opinion it is fully adequate, in scope and in quality, as a thesis for the degree of Master of Science.

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**SPIN-S ISING MODEL IN A MAGNETIC FIELD: AN EFFECTIVE-FIELD THEORY ANALYSIS**

**ABSTRACT**

A method in Ising models is presented within the framework of the effective field theory (EFT) with correlations. In the present theory, we have derived a set of linear equations by taking as a basis the thermal averages of a central spin and a perimeter spin at the site i, which is defined within spin identities and differential operator technique. By solving numerically the set of linear equations derived for the Ising system with coordination number q = 3, we have evaluated numerically all spin correlation functions without using a kind of decoupling approximation in the spin system under a longitudinal magnetic field. The effects of the external longitudinal magnetic field on the longitudinal magnetization, susceptibility, internal energy and specific heat (all of them are expressed in terms of spin correlation functions) are discussed in detail. Numerical results are performed and analyzed for the cases of spin -1/2 in a longitudinal magnetic field and spin -1 with crystal field in a longitudinal magnetic field, respectively on the honeycomb lattice. Furthermore, for the same lattice, the spin -1/2 and spin -1 systems with transverse field in a longitudinal magnetic field have investigated. A number of interesting phenomena, originating from the external field and temperature have been found.

**Keywords:** Honeycomb lattice, longitudinal magnetic field, transverse field, spin-s system, magnetic properties, classical spin sysytem

**MANYETİK ALANDA SPİN-S ISING MODEL: BİR EFEKTİF ALAN TEORİSİ VE ANALİZİ**

# ÖZ

Bu çalışmada, korelasyonlu efektif alan teorisi temel alınarak, Ising spin sistemleri için yeni bir efektif alan teorisi geliştirildi. Geliştirdiğimiz teoride, spin özdeşlikleri ve diferansiyel operotör tekniği ile tanımlanmış, i konumunda bulunan komşu spinlerin ve merkezi spinin termal ortalamaları temel alınarak, lineer eşitlikler kümesi türetilmiştir. En yakın komşu sayısı q =3 olan Ising sistemi için türettilmiş olan lineer eşitlikler kümesini sayısal olarak çözerek, dış manyetik alan altındaki spin sisteminde herhangi bir eşleme yaklaşımı(decoupling approximation) kullanılmadan bütün korelasyon fonksiyonları numerik olarak hesaplandı. Boyuna dış alanın, sistemin manyetizasyonu, duygunluğu, iç enerjisi ve öz ısısı(Sözü edilen bütün termodinamik nicelikler spin korelosyon fonksiyonları cinsinden ifade edilebilmektedir) üzerindeki etkileri ayrıntılı olarak tartışıldı. Sırası ile, bal peteği örgüsü üzerindeki spin -1/2 ve kristal alanlı spin -1 sitemleri için numerik sonuçlar hesaplandı ve analiz edildi. Ayrıca aynı örgü için, hem boyuna hem de enine bir manyetik alan içinde bulunan spin -1/2 ve spin -1 sistemleri incelendi. Dış alan ve sıcaklıktandan kaynaklan ilginç sonuçlar bulundu.

**Anahtar sözcükler :**Bal peteği örgü, boyuna magnetik alan, enine magnetik alan, spin-s sistemi, magnetik özellikler, klasik spin sistemi

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# CHAPTER ONE
# INTRODUCTION

The magnetic state of a substance is described by a quantity called the magnetization vector. The magnitude of the magnetization vector is equal to the magnetic moment per unit volume of the substance. The total magnetic field in a substance depends on both the applied (external) field and the magnetization of the substance

$$B = \mu_0(1+\chi)h \qquad \text{and} \qquad \mu_m = \mu_0(1+\chi)$$

where $\mu_0$ is the permeability of free space, $\chi$ is a dimensionless factor called the magnetic susceptibility, $h$ external field, $B$ total magnetic field, $\mu_m$ is called the magnetic permeability of the substance. If the sample is paramagnetic, $\chi$ is positive, in which case magnetization is in the same direction as external field. If the substance is diamagnetic, $\chi$ is negative, and magnetization is opposite external field. It is important to note that this linear relationship between magnetization and external field does not apply to ferromagnetic substances.

Susbtances may also be classified in terms of how their magnetic permeability $\mu_m$ compares with $\mu_0$ as follows:

| | |
|---|---|
| Paramagnetic | $\mu_m > \mu_0$ |
| Diamagnetic | $\mu_m < \mu_0$ |
| Ferromagnetic | $\mu_m >> \mu_0$ |

Since $\chi$ is very small for paramagnetic and diamagnetic substances. $\mu_m$ is nearly equal to $\mu_0$ in these cases. For ferromagnetic substances, however, $\mu_m$ is typically several thousand times larger than $\mu_0$.

Certain crystalline substances, whose atomic constituents have permanent magnetic dipole moments, exhibit strong magnetic effects called ferromagnetism. Examples of ferromagnetic substances include iron, cobalt, nickel, gadolinium, and dysprosium. Such substances contain atomic magnetic moments that tend to align parallel to each other even in a weak external magnetic field. Once the moments are aligned, the substance remains magnetized after the external field is removed. This permanent alignment is due to a strong coupling between neighboring moments, which can be understood only in quantum mechanical terms.

Paramagnetic substances have a positive but small suscebtibility which is due to the presence of atoms (or ions) with permanent magnetic dipole moments. These dipoles interact only weakly with each other and are randomly oriented in the absence of an external magnetic field. When the substance is placed in an external magnetic field, its atomic dipoles tend to line up with the field. However, this aligment process must compete with the effects of thermal motion, which tends to randomize the dipole orientations. Aluminum, calcium, chromium, lithium, magnesium, niobium, oxygen, platinum and tungsten are paramagnetic.

A diamagnetic substance is one whose atoms have no permanent magnetic dipole moment. When an external magnetic field is applied to a diamagnetic substance such as bismuth, silver, silicon, nitrogen, gold, diamond, copper, lead, a weak magnetic dipole moment is induced in the direction opposite the applied field. Although the effect of diamagnetism is present in all matter, it is weak compared to paramagnetism or ferromagnetism (Serway, 1982).

Magnetic properties have important industrial and electronic applications. Especially these properties used in siclotron, superconduting, controlled nuclear fusion researches, memory of computers, sound and T.V recorders... Besides magnetic properties are shown by certain classes of minerals or synthetic crystalline materials that lack a center of symmetry. Magnetism is an important diagnostic tool for a few minerals. Although only minerals that are strongly attracted to a magnetic field are considered to be magnetic, all matter has some magnetic properties, even though it may be too small to be detectable. This is because all matter is made up of moving charged particles (electrons and protons), whose motion sets up magnetic fields.

In statistical physics, there are a great deal of aproaches developed to explain magnetic properties. Heisenberg model, XY model, Potts model, Ising model and so on. Because of Ising model is more feasible than other methods, in this study we have calculated magnetic properties of the ferromagnetic system with two-dimensional by using effective field theory (EFT) with correlations in Ising model.

### 1.1 Spin Systems

The aim of this chapter is to describe some of the most fundamental models of cooperative behaviour. To model a physical system one route is to include, as realistically as possible, all the complicated many body interactions and try to obtain a quantitative prediction of the behaviour by solving Schrodinger's equation numerically. The other extreme is to write down the simplest possible model that still includes the essential physics and hope that it is tractable to analytic or precise numerical solution. The aim here is often to study universal behaviour or to gain a qualitative understanding of the physics governing the behaviour of a given class of materials.

It is the latter approach that we shall take here. Despite the apparent simplicity of the models, they show a rich mathematical structure and are in general diffucult or, more usually, impossible to solve exactly. Moreover, and perhaps surprisingly at first sight, they do provide valid and usefull representations of experimental systems.

It is conventional and convenient to use magnetic language and write the model Hamiltonians in terms of spin variables, although they will turn out to be applicable to many non-magnetic systems. In all the examples considered here the spins will lie on the sites *i* of a regular lattice. Three-dimensional lattices, such as simple cubic, body-centred cubic, and face-centred cubic, are familiar from conventional crystallography but we shall also be interested in lattices in two dimensions. (Yeomans,1992)

### 1.1.1 Ising Model

Ising's model mainly consist of a lattice of spins ( magnetic moments),which can assume only two orientations, $S = \pm 1$ with respect to the z-axis. In a ferromagnetic system, there is an interaction between neighboring spins, in contrast to a paramagnetic system, and the interaction is such that parallel spins correspond to an energy $-J$ and antiparallel spins to an energy $+J$. Since the exchange interaction decreases rapidly with distance, we need to consider only nearest neighbors in lattice. Since the parallel orientation of the spins is energetically favorable, this interaction leads to an enhanced parallel alignment of the spins. On the other hand, if the value of the exchange integral $J$ is negative, antiparallel alignment is preferred.

The Hamiltonian thus reads, at first without an external magnetic field:

$$H(S_1,\ldots,S_N) = -J\sum_{<i,j>} S_i S_j \qquad (1.1.1)$$

where one has to sum over all pairs of nearest neighbors. It is clear that the structure of the Hamiltonian depends on the coordination number q of the lattice (the number of nearest neighbors).

The Ising model and its various variants are of the most extensively studied many-body system. The reason is due to the fact that they can described fairly well numerous physical system, such as magnetic spin systems, binary alloys, lattice gas, and so on. The experimental examinations of magnetic spin systems under high longitudinal magnetic field have been studied for many years (Albertini et al, 2001; Doerr et al, 2001; Koyama et al, 2001) . These experimental results show that the longitudinal magnetic field has a strong influence on magnetic and thermodynamic properties of the system. Theoretically, in the literature, there is a few works which have been extended to the Ising system by taking into account the longitudinal magnetic field. Using the cluster variation method, C. Ekiz and M. Keskin (Ekiz & Keskin, 2003) studied the magnetic properties of the mixed spin -1/2 and spin -1 Ising ferromagnetic system with a crystal-field interaction in the absence and presence of an external field. Thermal variations of order parameters are investigated and the metastable and unstable branches of the order parameters are obtained besides the stable states. Wei et al. (Wei et al, 2004) have evaluated the magnetic properties of mixed Ising ferromagnetic system on the square lattice under a longitudinal magnetic field using the effective field theory(EFT) with correlations. They found some interesting results due to the applied external field. Magnetic properties of biaxial spin systems in a longitudinal magnetic field are studied using EFT with correlations (Jiang, Bai & Wei, 2005). The effects of the external longitudinal magnetic field on the longitudinal magnetization and susceptibility are discussed in detail. Wei Jiang and Bao-Dong Bai (Jiang & Bai, 2005) also studied the effects of the longitudinal magnetic field on the magnetic properties of the spin system with the crystal-field. They found a number of interesting phenomena due to the applied longitudinal magnetic field, such as, the shape of hysteresis loops and susceptibility are dependent on the longitudinal magnetic field and crystal field. In reference (Jiang & Bai, 2006), the influences of an external longitudinal magnetic field on the magnetic properties of mixed-spin -1/2 and spin -3/2 Ising ferromagnetic or ferrimagnetic bilayer systems is studied. The results show the longitudinal magnetic field plays an important role in the magnetic properties of the system.

The magnetic properties of the spin-S Ising system with crystal field and transverse field interaction in the absence of an external magnetic field are studied by using EFT with correlations (Jiang & Wei, 2000; Jiang, Wei & Xin, 2000; Jiang, Wei & Xin, 2000; Htoutou et al, 2004; Wei et al, 2001). At all of the studies mentioned above has been used a kind of decoupling approximation in EFT. The decoupling approximation neglects the correlations between different spins, which appear when expanding the identities. In a previous work , (Polat, Akıncı & Sökmen, 2003) have discussed the order parameters (magnetization, quadrupole moment, biquadrupole moment, and so on) and the phase diagrams of spin -1 Ising ferromagnetic systems (q = 3, 4 and 6) without using a kind of decoupling approximation in the spin system with crystal field and transverse field, respectively in the absence of a longitudinal magnetic field. The results show that the values of critical transverse field for the spin -1 transverse Ising systems improved those obtained by the pair approximation(Ma & Ma, 1993).

#### *1.1.1.1 Spin-1/2 Ising Model*

The system consist of the spins (i.e. particles which have non-zero magnetic moment about the spin) on a lattice. A general form of the S-1/2 Ising model's Hamiltonian is

$$H = -h\sum_{i} s_i - J\sum_{<i\,j>} s_i s_j - K\sum_{<i\,j\,k>} s_i s_j s_k - \ldots \tag{1.1.2}$$

where $s_i$ is the spin operator, $h$ is the magnetic field at a site $i$ and $J$, $K$, ... are exchange interactions which couple two, three ... spins. If one neglect the three and higher spin interactions the model is named next nearest Ising model etc.

Ising proposed his model in 1925 and solved it for a one dimensional system (Ising, 1925). (He didn't find any phase transition in one dimensional. After the physicists say the model has phase transition at absolute zero.) The free energy of the two dimensional zero field Ising model was first obtained by Onsager in 1944 (Onsager, 1944). He diagonalized the transfer matrix by irreducible represantations of a related matrix algebra. In 1949 his student Kaufman simplified this derivation by showing that the transfer matrix belongs to the group of spinor operators (Kaufman, 1949). A completely different technique was discovered by Kac and Ward in 1952 (Kac & Ward, 1952). They used combinatorial arguments to write the partition function as a determinant which could be easily evaluated. Hurst and Green (Hurst & Green, 1960) and Kasteleyn (Kasteleyn, 1963) also used combinatorial arguments. They write the partition function as a Pfaffian. Another combinatorial solution was obtained by Vdovichenko in 1964 (Vdovichenko, 1964). After then in 1978 Baxter and Enting have shown that the planar Ising models can be solved quite directly by using the star-triangle relations a recurrence relation(Baxter & Enting, 1964). Recently in 2000 Istrail showed that the three dimensional Ising model cannot be solved analytically (Istrail, 2000). Until now physicists have not reach the exact solution of the two dimensional Ising model with external field and three dimensional Ising model.

Beside all these there have been some approximated solutions, series expansions and some computer simulations. In 1907 Weiss explained the magnetic behavior of ferromagnetic domains with his mean molecular field theory. In 1934, 1935 Bragg and Williams developed the idea “the work expended in transferring an atom from a ordered position to a disordered one is directly proportional to the degree of order prevailing in the system” and they introduced the concept of long-range order (Bragg & Williams, 1934, Bragg & Williams, 1935 ). The mean field approach leads naturally to the Bethe approximation (Bethe, 1935). In 1936 Peierls was demonstrate that a sufficiently low temperatures the Ising model in two or three dimensions must exhibit a phase transition (Peierls, 1936).

#### *1.1.1.2 Spin-1 Ising Model*

For systems with more than two states higher-spin Ising models are appropriate. For example, the most general Hamiltonian for the spin-1 Ising model is

$$H = -J\sum_{<i,j>} s_i s_j - K\sum_{<i,j>} s_i^2 s_j^2 - D\sum_i s_i^2 - L\sum_{<i,j>} (s_i^2 s_j + s_i s_j^2) - h\sum_i s_i \qquad (1.1.3)$$

where $J$ is exchange interacion, the first summation is over the nearest-neighbor pair of spins and the operator $s_i$ takes the values of $s_i = \pm 1$ and 0, $K$ is quadrupole interactions, $D$ is a crystal-field anisotropy, $h$ represents the longitudinal magnetic field.

Because of its enlarged parameter space the spin-1 Ising model exhibits a much richer variety of critical behaviour than its spin-1/2 counterpart.

### *1.1.1.3 Analytic and Symmetry Properties of the Ising Model*

The nearest neighbor Ising model's Hamiltonian is

$$H = -J \sum_{<i,j>} s_i s_j - h \sum_i s_i \tag{1.1.4}$$

The magnetization per site is given by

$$M = -\frac{1}{N}\frac{\partial F}{\partial h} \tag{1.1.5}$$

The analytic properties of the Ising model's free energy is as follows:

1. $f < 0$
2. *f(h, J, T, ...)* is continuous.
3. $\partial f / \partial T$, $\partial f / \partial h$, ... exist almost everywhere.
4. The entropy per site $S = -\partial f / \partial T \geq 0$ almost everywhere.
5. $\partial f / \partial T$ is monotonically non-increasing with $T$ i.e. $\partial^2 f / \partial T^2 \leq 0$
6. $\partial f / \partial h$ is monotonically non-increasing with $h$ i.e. $\partial^2 f / \partial h^2 \leq 0$

The properties 5 and 6 implies that specific heat at constant magnetic field and the isothermal susceptibility are greater than (or equal to) zero.

$$C_h = -\frac{\partial^2 f}{\partial T^2}\Big|_h \;\geq\; 0$$

$$\chi_T = -\frac{\partial^2 f}{\partial h^2}\Big|_T \;\geq\; 0 \tag{1.1.6}$$

Proofs of the properties can be found in Goldenfeld, 1992.

By inspection one can show that

$$\sum_{\{s_i=\pm 1\}} \phi(\{s_i\}) = \sum_{\{s_i=\pm 1\}} \phi(\{-s_i\}) \tag{1.1.7}$$

where $\phi$ is the any function of the spin configuration. With this, two symmetry properties of the model is as follows

1. Time-reversal symmetry:

(1.1.4) implies that

$$H\,(\,h, J, \{\,s_i\,\}\,) = H\,(\,-h, J, \{-\,s_i\,\}\,) \tag{1.1.8}$$

The partition function is given by

$$Z[\{K_n\}] = Tre^{-\beta H} \tag{1.1.9}$$

where $\beta = 1/k_B T$ ($k_B$ is the Boltzmann constant and T is the absolute temperature). The operation *Tr* means sum over all degrees of freedom, or the sum including every possible value of each degree of freedom. The free energy is defined by

$$F\,[K_n] = -k_B T \log Z \tag{1.1.10}$$

from using (1.1.9) in (1.1.10) and with (1.1.8) one can show that

$$f\,(\,h, J, T\,) = f\,(\,-h, J, T\,) \tag{1.1.11}$$

e.g. the free energy is even in *h*.

2. Sublattice symmetry:

One can divide the lattice into two sub-lattice A and B, where $s_i^A$ are the spins in the sub-lattice A and $s_i^B$ are the spins in the sub-lattice B and $s_i^A$ are interacts only

$s_i^B$ (and vice versa). Under no magnetic field one can show that

$$H(0,-J,\{s_i^A\},\{s_i^B\}) = H(0,J,\{s_i^A\},\{-s_i^B\}) \qquad (1.1.12)$$

and it can be shown that this implies

$$f(0, J, T) = f(0, -J, T) \qquad (1.1.13)$$

this means that; in zero magnetic field, the ferromagnetic Ising model ($J > 0$) and the anti-ferromagnetic Ising model ($J < 0$) have the same thermodynamics.

The proofs can be found in Goldenfeld, 1992

#### *1.1.1.4 Importance of Thermodynamic Limit and Spontaneous Symmetry Breaking*

Magnetization is given by

$$M = -\frac{1}{N}\frac{\partial F(h)}{\partial h} \qquad (1.1.14)$$

From the time reversal symmetry $f(h, J, T) = f(-h, J, T)$

$$M = -\frac{1}{N}\frac{\partial F(h)}{\partial h} = -\frac{1}{N}\frac{\partial F(-h)}{\partial h} = \frac{1}{N}\frac{\partial F(-h)}{\partial(-h)} = -M(-h)$$

Thus

$$M(h) = -M(-h) \qquad (1.1.15)$$

At $h = 0$ we must have

$$M(0) = -M(0) = 0 \qquad (1.1.16)$$

This shows that the magnetization in zero external fields must be zero. But this is true only for finite systems. It fails in the thermodynamic limit, because *F (h)* can develop a discontinuity in its first derivative $\partial F(h)/\partial h$. Indeed (1.1.12) does not imply (1.1.17) unless one make the additional assumption that *F (h)* is smooth at $h = 0$ and its left and right derivatives are equal. These two conditions can be written as follows:

$$F(h) = F(0) + O(h^n) \tag{1.1.17}$$

where n>1 and

$$\lim_{\varepsilon \to 0} \frac{f(+\varepsilon) - f(0)}{\varepsilon} = \lim_{\varepsilon \to 0} \frac{f(-\varepsilon) - f(0)}{\varepsilon} = 0 \tag{1.1.18}$$

However none of the properties of *f ( h )* guarantee that smoothness. Instead of (1.1.17) one can write the *f ( h )* as follows :

$$F(h) = F(0) - M_S |h| + O(h^n) \tag{1.1.19}$$

where n>1. (1.1.19) is not differentiable at $h = 0$ but still satisfy the conditions of Ising model's free energy which are given above. Thus for spontaneous magnetization one can find

$$M_S = \lim_{h \to 0^+} -\frac{\partial f(h)}{\partial h}$$

$$-M_S = \lim_{h \to 0^-} -\frac{\partial f(h)}{\partial h} \tag{1.1.20}$$

$M_S$ is a function of temperature. At zero temperature $M_S$ should be unity. As the temperature rises toward $T_C$ the value of spontaneous magnetization is reduced, as an increasingly greater fraction of spins are flipped by thermal fluctuations. At $T_C$ the spontaneous magnetization has fallen to zero. This set of phenomena known as spontaneous symmetry breaking. $T_C$ is known as the critical point (Curie temperature).

### *1.1.1.5 Some Important Concepts*

In phase transitions (or critical phenomena) the concept of order parameter is very important. It is simply the measure of the order prevailing the system. For example for ferromagnetic systems the magnetization defines the order of the system then for ferromagnetic systems the order parameter is magnetization of the system. For ferrimagnetic and antiferromagnetic systems the order parameter is sublattice magnetizations, for ferroelectic systems condensate wave function and the superconductors ground state wave function.

The critical point is the point (temperature or some other coupling) that which the system change its phase.

Critical point exponents (or simply critical exponents) is used to explain the behaviour of the thermodynamic functions near the critical point. In general the critical point exponents defined as

$$\lambda = \lim_{t \to 0} \frac{\ln |F(t)|}{\ln |\ t\ |} \qquad (1.1.21)$$

where λ is the critical point exponent about the thermodynamic function *F(t)* and $t = \frac{T - T_c}{T_c}$ reduced temperature. It is more usually written

$$F(t) \sim |\mathrm{t}|^{\lambda} \qquad (1.1.22)$$

Equation (1.1.22) is explain the behaviour of the thermodynamic function *F(t)* near the critical point ($T_C$).

Some other important concept universality, it is classify the systems with three parameter: the dimensionality of the space in which the system is embedded, the number of the component of the order parameter of the system (dimensionality of the order parameter) and the range of microscopic interactions in the system (short ranged or long ranged) and universality asserts that the systems in same universality class have same critical behaviour. Although the thermodynamics of the systems depends on the specific values of the coupling constants in the Hamiltonian, type of the lattice and everything other, the critical behaviour does not depend on these details.

Thus when one can solve the system in one universality class and get the critical exponents about that system, one can explain in the critical behaviour of the other systems in the same universality class and get the critical exponents about them.

### *1.1.1.6 Extentions of the Ising Model and Importance of the Critical Phenomena*

Extensions of the Ising models are very common. For example, one can study the effects of disorder by assigning random values of $J$. When these values are fixed the model is called spin glass. In the random-field Ising model (Gofman et al., 1996), the values of the fields $H_i$ are assigned randomly at each site such that the mean of the $h$ is zero. A particularly interesting model is the anisotropic next-nearest–neighbor Ising model (ANNNI) (Bak & Boehm, 1980), for which the nearest-neighbor interactions are ferromagnetic, but the next-nearest–neighbor interactions are antiferromagnetic. Also of interest is the Blume-Emery-Giriffiths model (Blume et al., 1971), which is combination of a lattice gas and spin model. Here each site can have three values. This model was first used to model liquid $^3He-^4He$ mixtures.

The importance of the critical phenomena comes from the applications to the other systems such as polymers, liquid crystals, lattice gauge theories, chaos theory, percolation, fractals, disordered glassy systems, nonequilibrium driven systems, hydrodynamics, self-organized systems and some social systems.

### 1.1.2 The q-State Potts Model

Many different spin models, some driven by theoretical and some by experimental considerations, have been defined in the scientific literature. The only other classical spin model that I shall define here is the *q*-state Potts model. The relation of this system to the physisorption of krypton atoms on a graphite surface provides an interesting example of how to construct a model Hamiltonian with the correct symmetry.

To define the Potts model a *q*-state variable, $\alpha_i = 1, 2, 3 \ldots q$, is placed on each lattice site. The interaction between the spins is described by the Hamiltonian

$$H = -J \sum_{\langle i\, j \rangle} \delta_{\alpha_i\, \alpha_j} \tag{1.1.23}$$

$\delta$ is a Kronecker delta-function so the energy of two neighbouring spins is –*J* if they lie in the same state and zero otherwise. It is easy to convince oneself that the Potts model has *q* equivalent ground states where all the spins are identical but can take any one of the *q* values. As the temperature is increased there is a transition to a paramagnetic phase which is continuous for $q \le 4$ but first-order for $q > 4$ in two dimensions.

For *q*=2 the Potts model is identical to the spin-1/2 Ising model. Note, however, that for *q*=3 the Hamiltonian (1.1.23) does not correspond to the first term in eqn (1.1.3) because the three states of the spin-1 Ising model are not equivalent (Yeomans, 1992).

### 1.1.3 Heisenberg Model

The restriction of the Ising model is that the spin vector can only lie parallel to the direction of quantization introduced by the magnetic field. This means that the Ising Hamiltonian can only prove useful in describing a magnet which is highly anisotropic in spin space. There are physical systems, $MnF_2$ for example, which to a good approximation obey this criterion, but fluctuations of the spin away from the axis of quantization must inevitably occur to some degree.

A more realistic model of many magnets with localized moments is

$$H = -J_z \sum_{<i,j>} s_i^z s_j^z - J_\perp \sum_{<i,j>} (s_i^x s_j^x + s_i^y s_j^y) - h\sum_i s_i^z \tag{1.1.24}$$

where *x*, *y* and *z* label Cartesian axes in spin space. For $J_\perp = J_z$ (1.1.24) can be written

$$H = -J \sum_{<i,j>} \vec{s_i} . \vec{s_j} - h\sum_i s_i^z \tag{1.1.25}$$

This is the Heisenberg model.

The Heisenberg model was introduced in 1928 and was discussed in some detail as a model of ferromagnetism. It gives a reasonable description of the properties of some magnetic insulators, such as EuS, and provides a microscopic Hamiltonian describing the exchange interaction which leads to ferromagnetism. However, it does not include the possibility of non-localized spins and assumes complete isotropy in spin space.

The most fundamental theoretical difference between the Heisenberg and Ising models is that for the former the spin operators do not commute. Therefore it is a quantum mechanical rather than a classical spin model with corresponding greater difficulty in analytic or numerical treatments. Quantum models can be mapped on to classical spin systems in one higher dimension and there are some exact results for one-dimensional quantum models, just as for two-dimensional classical models. Moreover, just as the Ising model only has a finite temperature phase transition for $d > 1$, the Heisenberg model orders at zero temperature unless $d > 2$.

The classical limit of the Heisenberg model can be constructed by taking the number of spin components to infinity and normalizing the spin from $\sqrt{S(S+1)}$ to 1. The spins become three-dimensional classical vectors. This limit, which leads to considerable simplifications in theoretical work, is useful because the critical exponents of the classical and quantum Heisenberg models are the same. This is an example of universality (Yeomans, 1992).

### 1.1.4 XY Model

A second quantum mechanical spin model is the X-Y model, equation (1.1.24) obtained by putting $J_z = 0$ in the Hamiltonian

$$H = -J_{\perp} \sum_{<i,j>} (s_i^x s_j^x + s_i^y s_j^y) - h_x \sum_i s_i^x \tag{1.1.26}$$

This leads to spins which are two-dimensional, quantum mechanical vectors. The X-Y model, like the Heisenberg model, only has a conventional phase transition at non-zero temperature for $d > 2$. However, in $d = 2$ there is a transition at finite temperatures to an unusual ordered phase with quasi long-range order. This is marked by the correlations decaying algebraically for all temperatures, not just at the critical point itself (Yeomans, 1992).

# CHAPTER TWO
# DIFFERENTIAL OPERATOR TECHNIQUE

## 2.1 Callen Identity

The Hamiltonian of the spin-1/2 Ising system is

$$H = -J\sum_{<i\,j>} s_i s_j - h\sum_{i} s_i \tag{2.1.1}$$

where $J$ is the exchange interaction, $s_i$ is the spin operator's $z$ component at a site $i$, $h$ is the external magnetic field, $\beta = 1/k_B T$, $k_B$ is the Boltzmann constant, $T$ is the absolute temperature and < … > denotes the canonical ensemble average. The first sum runs over the distinct pairs of spins and the second one runs over $N$ identical spins. The partition function and the average (expectation) value of the spin variable at a site $i$ is

$$Z = Tre^{-\beta H} \tag{2.1.2}$$

$$\langle s_i \rangle = \frac{1}{Z} Trs_i.e^{-\beta H} \tag{2.1.3}$$

here Tr means the sum over the accessible states of the system. The exact relation for the average value of the spin variable can be derived from (2.1.3) and (2.1.2). For this purpose, the Hamiltonian is separate two part (which are commute each other). One part is about the $i$ th site and the other part does not depend on the site $i$.

$$H = H_i + H^l \tag{2.1.4}$$

with

$$H_i = -s_i . E_i \tag{2.1.5}$$

where

$$E_i = J \sum_{j=1}^{z} s_j + h \tag{2.1.6}$$

$E_i$ can be treated as an operator expressing the local field at a site *i*. Since the Hamiltonian and its two part are commute each other (because $\left[ s_i , s_j \right] = 0$ for $i \neq j$) (2.1.3) can be expressed as

$$< s_i >= \frac{1}{Z} \left\{ Tre^{-\beta H} \left[ \frac{tr_{(i)} s_i \exp(-\beta H_i)}{tr_{(i)} \exp(-\beta H_i)} \right] \right\} \tag{2.1.7}$$

where $tr_{(i)} = \sum_{i=1}^{-1}$ is the trace associated with the variable at a site *i*. By performing the partial trace

$$\left\langle s_i \right\rangle = \frac{1}{Z} \left\{ Tre^{-\beta H} \tanh(\beta E_i) \right\}$$

$$= < \tanh(\beta E_i) > \tag{2.1.8}$$

This is the Callen identity (Callen, 1963). The derivation of (2.1.8) can be generalized as follows

$$< \left\{ f_i \right\} s_i >=< \left\{ f_i \right\} \tanh(\beta E_i) > \tag{2.1.9}$$

where $\left\{ f_i \right\}$ can be any function of Ising variables except the site *i*. Furthermore, the above derivation of (2.1.8) can also be generalized the spin-S Ising systems then one obtains

$$<\left\{ f_i \right\} s_i^z >= S < \left\{ f_i \right\} B_s(\beta E_i) > \tag{2.1.10}$$

where $B_s(x)$ the Brillouin function

$$B_s(x) = \frac{2S+1}{2S}\coth\left(\frac{2S+1}{2S}x\right) - \frac{1}{2S}\coth\left(\frac{x}{2S}\right) \tag{2.1.11}$$

(2.1.10) is the exact relation for the average magnetization of the Ising system. But it's hard to evaluate this exact relation for the systems z = 3,4,6,10...

First approach to Callen identity was introduced by Matsudai and he noticed the following exact relations which are valid for S-1/2 systems (Matsudai, 1973)

$$\tanh(Ks_1) = As_1, \qquad A = \tanh(K)$$

$$\tanh(Ks_1 + Ks_2) = B(s_1 + s_2), \qquad B = \frac{1}{2}\tanh(2K)$$

$$\tanh(Ks_1 + Ks_2 + Ks_3) = C_1(s_1 + s_2 + s_3) + C_2(s_1 s_2 s_3),$$

$$C_1 = \frac{1}{4}(\tanh(3K) + \tanh(K)),$$

$$C_2 = \frac{1}{4}(\tanh(3K) - \tanh(K)) \tag{2.1.12}$$

Similar relations can be expressed for higher number of spins. (But it is rather diffucult for the higher spin Ising systems). Instead of this, in 1979 Honmura and Kaneyoshi introduced the differential operator technique and with this technique they easily achieved this relations. (Honmura & Kaneyoshi, 1979)

## 2.2 Differential Operator Technique

The exponential differential operator acts the function of *x* and it gives;

$$e^{a\nabla} f(x) = f(x+a) \tag{2.2.1}$$

where $a$ is a constant, $\nabla = \partial / \partial x$ differential operator and $f(x)$ is an arbitrary function of *x*. This can be seen with expanding the exponential term in Taylor series

$$e^{a\nabla} f(x) = [1 + a\nabla + \frac{a^2}{2!}\nabla^2 + ...] f(x) = f(x) + a\nabla f(x) + \frac{a^2}{2!}\nabla^2 f(x) + ... = f(x+a)$$

Thus, the (2.1.9) and (2.1.10) can be written in a new form with using (2.2.1)

$$<\{f_i\} s_i> = <\{f_i\} \tanh(\beta E_i)> = <\{f_i\} e^{E_i \nabla} \tanh(\beta x)\big|_{x=0}> \tag{2.2.2}$$

$$<\{f_i\} s_i^z> = S <\{f_i\} B_S(\beta E_i)> = S <\{f_i\} e^{E_i \nabla} B_S(\beta x)|_{x=0}> \tag{2.2.3}$$

Since the functions in the ensemble average are independent of this average, they can go outside the ensemble average bracket

$$<\{f_i\} s_i> = <\{f_i\} e^{E_i \nabla}> \tanh(\beta x)\big|_{x=0} \tag{2.2.4}$$

$$<\{f_i\} s_i^z> = S <\{f_i\} e^{E_i \nabla}> B_S(\beta x)\big|_{x=0} \tag{2.2.5}$$

(2.2.4) and (2.2.5) can be written in general

$$<\{f_i\} s_i> = <\{f_i\} e^{E_i \nabla}> f(x)\big|_{x=0} \tag{2.2.6}$$

(2.2.6) is the fundamental relation of the differential operator technique and this is an exact relation for the system. $f(x)$ may be given by (Jiang et al., 2000);

$$f(x)=\frac{1}{\sum_{n=1}^{m}\exp(\beta\lambda_n)}\left\{\sum_{n=1}^{m}<\varphi_n\left|S_i^z\right|\varphi_n>\exp(\beta\lambda_n)\right\} \tag{2.2.7}$$

where $\lambda_n$ are the eigenvalues of $-H_i$ and $\varphi_n$ are their corresponding eigenvectors. $H_i$ is Hamiltonian about the $i$ th spin (which includes the terms containing $i$ th spin) on the lattice. If one wants to compute the average of the different component of the spin $i$ then must change $S_i^z$ in (2.2.7) to that component's matrix representation. Thus $f(x)$ depends on the system as well as the fields acts on the system.

Average magnetizations, critical temperatures, internal energies, susceptibilities and specific heats can be computed with the differential operator technique then one can gain the phase diagrams of the different systems. (2.2.6) is exact relation for the Ising system but for evaluating (2.2.6) one needs make some approximations. (2.2.6) can give MFA and Zernike approximation's results. (Kaneyoshi, 1993) Beside this, from (2.2.6) one can gain the results which are the same as the Bethe-Pierls approximation's results (which is the best approximation for the Ising systems as far as we know). But although to apply Bethe-Pierls approximation technique to higher spin Ising systems. (2.2.6) can evaluate with the expanding the exponential differential operator in terms of the hyperbolic trigonometric functions. For instance for S-1/2 and S-1 Ising system, the exponential differential operator can be written as with using Van der Waerden identity respectively ($a$ is an arbitrary constant)

$$\begin{aligned} e^{as_i} &= \cosh(a/2)+2s_i\sinh(a/2), && s_i=\pm\frac{1}{2} \\ e^{as_i} &= (s_i)^2\cosh(a)+s_i\sinh(a)+1-(s_i)^2, && s_i=\pm1,0 \end{aligned} \tag{2.2.8}$$

For higher spin Ising systems these identities becomes more complex and one need to use the approximated Van der Waerden identity. (Tucker, 1994)

**2.3 Spin-S Systems**

We can take any spin ( $s_0$ ) and it's z nearest neighbors ( $s_\delta$ ) in the system and form a cluster. From (2.2.6) we get for the central spin in the cluster

$$<\{f_0\}s_0>=<\{f_0\}e^{E_0\nabla}>f(x)\Big|_{x=0} \tag{2.3.1}$$

and for the perimeter spin in the cluster

$$<\{f_\delta\}s_\delta>=<\{f_\delta\}e^{E_\delta\nabla}>f(x)\Big|_{x=0} \tag{2.3.2}$$

we get the above equations. Here $E_0 = J\sum_{\delta=1}^{z} s_\delta$ and $E_\delta = J\sum_{j=1}^{z} s_{\delta+j}$ where z is the number of the nearest neighbor spins in the lattice, $\{f_\delta\}$ is the any function of the spin variable except $s_\delta$ and $\{f_0\}$ is the any function of the spin variable except $s_0$. Instead putting the interactions of the perimeter spin's nearest neighbor spins in the (2.3.2) one can treat this interactions as an effective field. Thus we have two interactions of the perimeter spin in the (2.3.2); one is the interaction of the perimeter spin with the neighbor spins outside the cluster. The latter is treated with an effective field. (A)

$$E_\delta = J\sum_{j=1}^{z} s_{\delta+j} = Js_0 + J\sum_{\substack{j=1 \\ j\neq-\delta}}^{z} s_{\delta+j} = Js_0 + (z-1)A \tag{2.3.3}$$

where $A$ is the effective field per perimeter spin.

If we insert (2.3.3) in the (2.3.2) and $E_0$ in the (2.3.1) we get the following equations for the central and the perimeter spin's average magnetizations :

$$< \{ f_0 \} s_0 > = < \{ f_0 \} e^{J \sum_{\delta=1}^{z} s_\delta \nabla} > f(x) \Big|_{x=0}$$

$$= < \{ f_0 \} \prod_{\delta=1}^{z} e^{J s_\delta \nabla} > f(x) \Big|_{x=0} \tag{2.3.4}$$

$$< \{ f_\delta \} s_\delta > = < \{ f_\delta \} e^{(J s_0 + (z-1)A)\nabla} > f(x) \Big|_{x=0}$$

$$= < \{ f_\delta \} e^{J s_0 \nabla} > f(x+\alpha) \Big|_{x=0} \tag{2.3.5}$$

where $\alpha = (z-1)A$. These are valid for spin-S Ising systems.

## CHAPTER THREE
## SOLUTIONS WITHOUT DECOUPLING APPROXIMATION

### 3.1 Solutions of Spin-1/2 Ising Ferromagnetic System in a Longitudinal Magnetic Field

At first, we discuss how the theory can be formulated within the framework of the effective field with correlations. To do this, we consider a lattice with two dimensional which is consisted of $N$ identical spins arranged. On the lattice, we select a system which consists a central spin, labeled $0$, and $q$ perimeter spins being the nearest – neighbors of the central spin. The system consists of $(q+1)$ spins being independent of the value of $S$. The nearest-neighbor spins are in an effective field produced by the outer spins, which can be determined by the condition that the thermal average of the central spin is equal to that of its nearest-neighbor spins. The Hamiltonian of the spin-S(S-1/2) system in a longitudinal magnetic field is given by

$$H = -J\sum_{<i,j>} S_i^z S_j^z - h\sum_i S_i^z \tag{3.1.1}$$

where, the first summation is over the nearest-neighbor pair of spins and the operator $S_i^z$ takes the values of $S_i^z = \pm\frac{1}{2}$. $h$ represents the longitudinal magnetic field. By the use of the exact Van der Waerden identity (Balcerzak, 2002; Callen, 1963; Suzuki, 1965) for the spin -1/2 Ising ferromagnetic system with the coordination number $q$, the thermal average of the spin variables at the site $i$ is given by

$$\left\langle \{f_i\} S_i^z \right\rangle = \left\langle \{f_i\} \exp( J\sum_{\delta}^{z} S_\delta^z)\nabla \right\rangle F\ (x)\Big|_{x=0} \tag{3.1.2}$$

where, $\beta = 1/k_B T$, with $T$ the absolute temperature, $k_B$ is the Boltzmann constant, $\nabla = \partial/\partial x$ is a differential operator, $\delta$ expresses the nearest-neighbor sites of the central spin and $\{f_i\}$ can be any function of the Ising variables as long as it is not a function of the site. From (3.1.2) with $\{f_i\}=1$, the thermal average of a central spin can be represented in the form for honeycomb ($q$ = $3$) lattice

$$m_0 = \left\langle S_0^z \right\rangle = \left\langle \prod_{\delta=1}^{3} [\cosh(\frac{1}{2}\ J\ \nabla) + 2S_i^z \sinh(\frac{1}{2}\ J\ \nabla)] \right\rangle F\ (x)\big|_{x=0} \qquad (3.1.3)$$

$$= u_0 + 6k_1 \langle S_1 \rangle + 12u_1 \langle S_1 S_2 \rangle + 8k_2 \langle S_1 S_2 S_3 \rangle \qquad (3.1.4)$$

with

$$u_0 = \cosh^3(\frac{1}{2}\ J\ \nabla)\, F(x)\big|_{x=0} \quad ,$$

$$u_1 = \sinh^2(\frac{1}{2}\ J\ \nabla) \cosh(\frac{1}{2}\ J\ \nabla)\, F(x)\big|_{x=0} \quad ,$$

$$k_1 = \sinh\ (\frac{1}{2}\ J\ \nabla) \cosh^2(\frac{1}{2} J\nabla) F(x)\Big|_{x=0} \quad ,$$

$$k_2 = \sinh^3(\frac{1}{2}\ J\ \nabla)\, F(x)\big|_{x=0} \quad .$$

where the coefficients $u_0, u_1, k_1$ *and* $k_2$ can be calculated from a mathematical identity $\exp(\alpha\ \nabla)F(x) = F(x+\alpha)$. The function $F\ (x)$ for spin – 1/2 Ising system is given by

$$F(x) = \frac{1}{2}\tanh(\frac{1}{2}\beta(x+h)) \ . \tag{3.1.5}$$

Next, the average value of a perimeter-spin in the system can be written as follow and it is found as

$$\begin{aligned} m_1 &= \left\langle S_\delta^z \right\rangle \\ &= \left\langle \exp( J \ S_0^z + (q-1) \ A)\nabla \right\rangle F(x)\big|_{x=0} \\ &= \left\langle [\cosh(\frac{1}{2} J\nabla) + 2S_\delta^z \sinh(\frac{1}{2} J\nabla)] \right\rangle F(x+\gamma)\big|_{x=0} \end{aligned} \tag{3.1.6}$$

$$< S_1 >= a_1 + a_2 < S_0 > \tag{3.1.7}$$

with

$$a_1 = \cosh(\frac{1}{2} \ J \ \nabla) F(x+\gamma)\big|_{x=0} \quad ,$$

$$a_2 = 2\sinh(\frac{1}{2} \ J \ \nabla) F(x+\gamma)\big|_{x=0}$$

where δ expresses the nearest-neighbor sites of the central spin, $\gamma = (q-1)A$ is the effective field produced by the (q – 1) spins outside the system and $A$ is an unknown parameter to be determined self-consistently.

When the right hand side of (3.1.3) and (3.1.6) is expanded, the multispin correlation functions may be obtained. The simplest approximation, and one of the most frequently adopted, for their treating is based on introducing the following decoupling approximation ( Tamura & Kaneyoshi, 1981):

$$\langle S_i^z S_j^z \cdots S_l^z \rangle \cong \langle S_i^z \rangle \langle S_j^z \rangle \cdots \langle S_l^z \rangle \tag{3.1.8}$$

for $i \neq j \neq \cdots \neq l$. The main difference of the method used in this study, in comparison with any decoupling approximation can be seen in the expanding of the right hand side of (3.1.3) and (3.1.6).

For the spin – 1/2 Ising system with $q$ = 3, taking as a basis (3.1.4) and (3.1.7), we have derived the set of linear equations of the spin correlation functions which interact in the system. It has been considered that (i) the correlations are depended only on the distance between the spins, (ii) the averaged value of a central spin and its nearest-neighbor spin (it is labeled as the perimeter spin) is equal to each other, and (iii) in the matrix representations of spin operator $\hat{S}$, the spin -1/2 system has the property $(S_i^z)^2 = 1/4$. Thus, the number of the set of linear equations obtained for the spin – 1/2 Ising system with $q$ = 3 reduce to six linear equations:

$$\langle S_0 \rangle = u_0 + 6k_1 \langle S_1 \rangle + 12u_1 \langle S_1 S_2 \rangle + 8k_2 \langle S_1 S_2 S_3 \rangle \quad ,$$

$$\langle S_1 \rangle = a_1 + a_2 \langle S_0 \rangle \quad ,$$

$$\langle S_1 S_0 \rangle = \frac{1}{2}k_1 + (u_0 + 2u_1)\langle S_1 \rangle + (4k_1 + 2k_2)\langle S_1 S_2 \rangle + 4u_1 \langle S_1 S_2 S_3 \rangle \quad ,$$

$$\langle S_1 S_2 S_0 \rangle = \frac{1}{4}u_1 + (k_1 + \frac{1}{2}k_2)\langle S_1 \rangle + (u_0 + 2u_1)\langle S_1 S_2 \rangle + 2k_1 \langle S_1 S_2 S_3 \rangle \ ,$$

$$\langle S_1 S_2 \rangle = a_1 \langle S_1 \rangle + a_2 \ \langle S_1 S_0 \rangle \quad ,$$

$$\langle S_1 S_2 S_3 \rangle = a_1 \langle S_1 S_2 \rangle + a_2 \left\langle S_1 S_2 S_0 \right\rangle \quad . \tag{3.1.9}$$

If (3.1.9) is written in the form of a $6 \times 6$ matrix and solved in terms of variables $x_i$ [ ( $i = 1, 2, 3, ..., 6$ ) ( *e. g.* , $x_1 = \langle S_0 \rangle$, $x_2 = \langle S_1 \rangle$, ..., $x_6 = \langle S_1 S_2 S_3 \rangle$ )] of the linear equations, all of the spin correlation functions can be determined easily as a function of the temperature and the longitudinal magnetic field which the other studies in the literature does not include. Since the thermal average of the central spin is equal to that of its nearest-neighbor spins within the present method, the unknown parameter *A* can be determined numerically by the relation

$$\langle S_0 \rangle = \langle S_1 \rangle, \text{ or } x_1 = x_2 \ . \tag{3.1.10}$$

By solving (3.1.10) numerically, for fixed values of *h/J*, we have obtained the parameter *A*. Then, we used the numerical values of *A* to obtain the spin correlation functions $\langle S_0 \rangle$, $\langle S_1 S_0 \rangle$, $\langle S_1 S_2 S_0 \rangle$, and so on.

### 3.2 Solutions of Spin-1 Ising Ferromagnetic System in a Longitudinal Magnetic Field with Crysal Field

The Hamiltonian of the spin-S( $S \geq 1$) system with crystal-field in a longitudinal magnetic field is given by

$$H = -J \sum_{<i,j>} S_i^z S_j^z - D \sum_i (S_i^z)^2 - h \sum_i S_i^z \tag{3.2.1}$$

where $D$ is a crystal-field anisotropy, the first summation is over the nearest-neighbor pair of spins and the operator $S_i^z$ takes the values of $S_i^z = \pm 1$ and $0$. $h$ represents the longitudinal magnetic field. By the use of the exact Van der Waerden identity (Balcerzak, 2002; Callen, 1963; Suzuki, 1965) for the spin -1 Ising ferromagnetic system with the coordination number *q*, the thermal average of the spin variables at the site $i$ is given by

$$\left\langle \{f_i\} S_i^z \right\rangle = \left\langle \{f_i\} \exp( J \sum_{\delta}^{z} S_\delta^z ) \nabla \right\rangle F\ (x)\Big|_{x=0} \tag{3.2.2}$$

where, $\beta = 1/k_B T$, with $T$ the absolute temperature, $k_B$ is the Boltzmann constant, $\nabla = \partial/\partial x$ is a differential operator, $\delta$ expresses the nearest-neighbor sites of the central spin and $\{f_i\}$ can be any function of the Ising variables as long as it is not a function of the site. From (3.2.2) with $\{f_i\} = 1$, the thermal average of a central spin can be represented in the form for honeycomb ($q$ = $3$) lattice

$$m_0 = \left\langle S_0^z \right\rangle = \left\langle \prod_{\delta=1}^{3} [1 + S_\delta^z \sinh(J\nabla) + (S_\delta^z)^2 \{\cosh(J\nabla) - 1\}] \right\rangle F\ (x)\Big|_{x=0} \tag{3.2.3}$$

$$\begin{aligned} &= l_0 + 3k_1 \langle S_1 \rangle + 3(l_1 - l_0)\langle S_1^2 \rangle + 3l_2 \langle S_1 S_2 \rangle + 6(k_2 - k_1)\langle S_1 S_2^2 \rangle + \\ &3(l_0 - 2l_1 + l_3)\langle S_1^2 S_2^2 \rangle + \ k_3 \langle S_1 S_2 S_3 \rangle + 3(l_4 - l_2)\langle S_1 S_2 S_3^2 \rangle + \\ &(k_1 - 2k_2 + k_4)\langle S_1 S_2^2 S_3^2 \rangle + (-l_0 + 3l_1 - 3l_3 + l_5)\langle S_1^2 S_2^2 S_3^2 \rangle \end{aligned} \tag{3.2.4}$$

with

$$l_0 = F(0),$$

$$l_1 = \cosh(J\nabla)\, F(x)\Big|_{x=0},$$

$$l_2 = \sinh^2(J\nabla)\, F(x)\Big|_{x=0},$$

$$l_3 = \cosh^2(J\nabla)\, F(x)\Big|_{x=0},$$

$$l_4 = \sinh^2(J\nabla) \cosh(J\nabla)\, F(x)\Big|_{x=0},$$

$$l_5 = \cosh^3(J\nabla)\, F(x)\Big|_{x=0},$$

$$k_1 = \sinh(J\ \nabla)\, F(x)\big|_{x=0} \quad ,$$

$$k_2 = \sinh(J\ \nabla)\cosh(J\ \nabla)\, F(x)\big|_{x=0} \quad ,$$

$$k_3 = \sinh^3(J\ \nabla)\, F(x)\big|_{x=0} \quad ,$$

$$k_4 = \sinh(J\ \nabla)\cosh^2(J\ \nabla)\, F(x)\big|_{x=0} \quad ,$$

where the coefficients $l_0, l_1, l_2, l_3, l_4, l_5, k_1, k_2, k_3$ and $k_4$ can be calculated from a mathematical identity $\exp(\alpha\,\nabla)\, f(x) = f(x+\alpha)$. The function $F(x)$ for spin $-$ 1 Ising system is given by

$$F\ (x) = \frac{2\sinh[\beta(x+h)]}{2\cosh[\beta\,(x+h)] + \exp(-\beta\, D)} \tag{3.2.5}$$

Next, the average value of a perimeter-spin in the system can be written as follow and it is found as

$$\begin{aligned} m_1 &= \left\langle S_\delta^z \right\rangle \\ &= \left\langle \exp(J\ S_0^z + (q-1)\ A)\nabla \right\rangle F(x)\big|_{x=0} \\ &= \left\langle [1 + S_0^z \sinh(J\ \nabla) + (S_0^z)^2\{\cosh(J\ \nabla) - 1\}] \right\rangle F(x+\gamma)\big|_{x=0} \end{aligned} \tag{3.2.6}$$

$$< S_1 >= (1 - < S_0^2 >)\ a_1 + < S_0 >\ a_2 + < S_0^2 >\ a_3 \tag{3.2.7}$$

with

$$a_1 = F(\gamma)\ \ ,$$

$$a_2 = \sinh(J\,\nabla)\,F(x+\gamma)\big|_{x=0} \quad ,$$

$$a_3 = \cosh(J\,\nabla)\,F(x+\gamma)\big|_{x=0} \quad ,$$

where $\gamma = (q-1)A$ is the effective field produced by the (q – 1) spins outside the system and $A$ is an unknown parameter to be determined self-consistently.

In contrast to the spin-$\frac{1}{2}$ Ising model, we have to introduce the additional parameters, $\left\langle (S_\delta^z)^2 \right\rangle$ and $\left\langle (S_0^z)^2 \right\rangle$, resulting from the usage of the Van der Waerden identity for the spin -1:

$$\left\langle (S_0^z)^2 \right\rangle = \left\langle \prod_{\delta=1}^{3} [1 + S_\delta^z \sinh(J\,\nabla) + (S_\delta^z)^2 \{\cosh(J\,\nabla) - 1\}] \right\rangle G(x)\big|_{x=0} \qquad (3.2.8)$$

$$\begin{aligned} \left\langle S_0^2 \right\rangle = {} & r_0 + 3n_1\langle S_1\rangle + 3(r_1 - r_0)\langle S_1^2\rangle + 3r_2\langle S_1S_2\rangle + 6(n_2 - n_1)\langle S_1S_2^2\rangle + \\ & 3(r_0 - 2r_1 + r_3)\langle S_1^2S_2^2\rangle + n_3\langle S_1S_2S_3\rangle + 3(r_4 - r_2)\langle S_1S_2S_3^2\rangle + \\ & 3(n_1 - 2n_2 + n_4)\langle S_1S_2^2S_3^2\rangle + (-r_0 + 3r_1 - 3r_3 + r_5)\langle S_1^2S_2^2S_3^2\rangle \end{aligned} \qquad (3.2.9)$$

with

$$n_1 = \sinh(J\nabla)\,G(x)\big|_{x=0}\,,$$

$$n_2 = \sinh(J\nabla)\cosh(J\nabla)\,G(x)\big|_{x=0}\,,$$

$$n_3 = \sinh^3(J\nabla)\,G(x)\big|_{x=0}\,,$$

$$n_4 = \sinh(J\nabla)\cosh^2(J\nabla)\,G(x)\big|_{x=0}\,,$$

$$r_0 = G(0) \quad ,$$

$$r_1 = \cosh(J\ \nabla)\, G(x)\big|_{x=0} \quad ,$$

$$r_2 = \sinh^2(J\ \nabla)\, G(x)\big|_{x=0} \quad ,$$

$$r_3 = \cosh^2(J\ \nabla)\, G(x)\big|_{x=0} \quad ,$$

$$r_4 = \sinh^2(J\ \nabla)\cosh(J\ \nabla)\, G(x)\big|_{x=0} \quad ,$$

$$r_5 = \cosh^3(J\ \nabla)\, G(x)\big|_{x=0} \quad .$$

where the function $G(x)$ is defined by

$$G(x) = \frac{2\cosh[\beta(x+h)]}{2\cosh[\beta(x+h)] + \exp(-\beta D)} \tag{3.2.10}$$

Corresponding to (3.2.6),

$$\left\langle (S_\delta^z)^2 \right\rangle = \left\langle [1 + S_0^z \sinh(J\ \nabla) + (S_0^z)^2 \{\cosh(J\ \nabla) - 1\}] \right\rangle G(x+\gamma)\big|_{x=0} \tag{3.2.11}$$

$$< S_1^2 > \ = (1 - < S_0^2 >)\ b_1 + < S_0 >\ b_2 + < S_0^2 >\ b_3 \tag{3.2.12}$$

with

$$b_1 = G(\gamma) \quad ,$$

$$b_2 = \sinh(J\ \nabla)\, G(x+\gamma)\big|_{x=0} \quad ,$$

$$b_3 = \cosh(J\ \nabla)\, G(x+\gamma)\big|_{x=0} \quad ,$$

When the right hand side of (3.2.3), (3.2.6), (3.2.8) and (3.2.11) is expanded, the multispin correlation functions may be obtained. The simplest approximation, and one of the most frequently adopted, for their treating is based on introducing the following decoupling approximation ( Tamura & Kaneyoshi, 1981):

$$\langle S_i^z (S_j^z)^2 \cdots S_l^z \rangle \cong \langle S_i^z \rangle \ \langle (S_j^z)^2 \rangle \cdots \langle S_l^z \rangle \qquad (3.2.13)$$

for $i \neq j \neq \cdots \neq l$. The main difference of the method used in this study, in comparison with any decoupling approximation can be seen in the expanding of the right hand side of (3.2.3), (3.2.6), (3.2.8) and (3.2.11).

For the spin – 1 Ising system with $q$ = 3, taking as a basis (3.2.4), (3.2.7), (3.2.9) and (3.2.12), we have derived the set of linear equations of the spin correlation functions which interact in the system. It has been considered that (i) the correlations are depended only on the distance between the spins, (ii) the averaged value of a central spin and its nearest-neighbor spin (it is labeled as the perimeter spin) is equal to each other, and (iii) in the matrix representations of spin operator $\hat{S}$, the spin -1 Ising system has the properties $(S_\delta^z)^3 = S_\delta^z$ and $(S_\delta^z)^4 = (S_\delta^z)^2$. Thus, the number of the set of linear equations obtained for the spin – 1 Ising system with $q$ = 3 reduce to twenty one linear equations:

$$\left\langle S_0^z \right\rangle = l_0 + 3k_1\langle S_1\rangle + 3(l_1 - l_0)\langle S_1^2\rangle + 3l_2\langle S_1S_2\rangle + 6(k_2 - k_1)\langle S_1S_2^2\rangle + 3(l_0 - 2l_1 + l_3)\langle S_1^2S_2^2\rangle +$$

$$k_3\langle S_1S_2S_3\rangle + 3(l_4 - l_2)\langle S_1S_2S_3^2\rangle + (k_1 - 2k_2 + k_4)\langle S_1S_2^2S_3^2\rangle + (-l_0 + 3l_1 - 3l_3 + l_5)\langle S_1^2S_2^2S_3^2\rangle,$$

$$\left\langle S_1S_0 \right\rangle = l_0\langle S_0\rangle + 3k_1\langle S_1S_2\rangle + 3(-l_1 + l_2 - l_3)\langle S_1S_2^2\rangle + 6(k_2 - k_1)\langle S_1^2S_2^2\rangle + k_3\langle S_1S_2S_3^2\rangle +$$

$$(-l_0 + 3l_1 - 3l_3 + 3l_4 + l_5)\langle S_1\, S_2^2S_3^2\rangle + \ (k_1 - 2k_2 + k_4)\langle S_1^2S_2^2S_3^2\rangle,$$

$$\left\langle S_1S_2S_0\right\rangle = (l_0-3l_1+3l_2-3l_3)\langle S_1S_2\rangle + (6k_2-3k_1)\langle S_1\,S_2^2\rangle + k_3\langle S_1S_2S_3^2\rangle +$$

$$(-l_0+3l_1-3l_2-3l_3+3l_4+l_5)\langle S_1\,S_2S_3^2\rangle + \ (k_1-2k_2+k_3+k_4)\langle S_1\,S_2^2S_3^2\rangle,$$

$$\left\langle S_1\right\rangle = a_1 + a_2\langle S_0\rangle + (a_3-a_1)\langle S_0^2\rangle,$$

$$\left\langle S_1\,S_2\right\rangle = a_1\langle S_1\rangle + a_2\langle S_1S_0\rangle + (a_3-a_1)\langle S_1S_0^2\rangle,$$

$$\left\langle S_1S_2S_3\right\rangle = a_1\langle S_1S_2\rangle + a_2\langle S_1S_2S_0\rangle + (a_3-a_1)\langle S_1S_2S_0^2\rangle,$$

$$\left\langle S_1^2\right\rangle = b_1 + b_2\langle S_0\rangle + (b_3-b_1)\langle S_0^2\rangle,$$

$$\left\langle S_1S_2^2\right\rangle = b_1\langle S_1\rangle + b_2\langle S_1S_0\rangle + (b_3-b_1)\langle S_1S_0^2\rangle,$$

$$\left\langle S_1^2S_2^2\right\rangle = b_1\langle S_1^2\rangle + b_2\langle S_0S_1^2\rangle + (b_3-b_1)\langle S_1^2S_0^2\rangle,$$

$$\left\langle S_0S_1^2\right\rangle = b_3\langle S_0\rangle + b_2\langle S_0^2\rangle,$$

$$\left\langle S_0S_1S_2^2\right\rangle = b_3\langle S_1S_0\rangle + b_2\langle S_1S_0^2\rangle,$$

$$\left\langle S_0S_1^2S_2^2\right\rangle = b_3\langle S_0S_1^2\rangle + b_2\langle S_1^2S_0^2\rangle,$$

$$\left\langle S_1S_2S_3^2\right\rangle = b_1\langle S_1S_2\rangle + b_2\langle S_1S_2S_0\rangle + (b_3-b_1)\langle S_1S_2S_0^2\rangle,$$

$$\left\langle S_1S_2^2S_3^2\right\rangle = b_1\langle S_1S_2^2\rangle + b_2\langle S_0S_1S_2^2\rangle + (b_3-b_1)\langle S_1S_2^2S_0^2\rangle,$$

$$\left\langle S_1^2S_2^2S_3^2\right\rangle = b_1\langle S_1^2S_2^2\rangle + b_2\langle S_0S_1^2S_2^2\rangle + (b_3-b_1)\langle S_1^2S_2^2S_0^2\rangle,$$

$$\left\langle S_0^2\right\rangle = r_0 + 3n_1\langle S_1\rangle + 3(r_1-r_0)\langle S_1^2\rangle + 3r_2\langle S_1S_2\rangle + 6(n_2-n_1)\langle S_1S_1^2\rangle + 3(r_0-2r_1+r_3)\langle S_1^2S_1^2\rangle +$$

$$n_3\langle S_1S_2S_3\rangle + 3(r_4-r_2)\langle S_1S_2S_3^2\rangle + 3(n_1-2n_2+n_4)\langle S_1S_2^2S_3^2\rangle +$$

$$(-r_0+3r_1-3r_3+r_5)\langle S_1^2S_2^2S_3^2\rangle,$$

$$\left\langle S_1 S_0^2 \right\rangle = (3r_1 - 2r_0)\langle S_1 \rangle + 3n_1\langle S_1^2 \rangle + 3(r_0 - 2r_1 + r_2 + r_3)\langle S_1 S_1^2 \rangle + n_3\langle S_1 S_2 S_3^2 \rangle +$$

$$3(r_4 - r_2)\langle S_1 S_2 S_3^2 \rangle + (-r_0 + 3r_1 - 3r_2 - 3r_3 + 3r_4 + r_5)\langle S_1 S_2^2 S_3^2 \rangle +$$

$$3(n_1 - 2n_2 + n_4)\langle S_1^2 S_2^2 S_3^2 \rangle,$$

$$\left\langle S_1^2 S_0^2 \right\rangle = 3n_1\langle S_1 \rangle + (3r_1 - 2r_0)\langle S_1^2 \rangle + 3(r_0 - 2r_1 + r_2 + r_3)\langle S_1^2 S_1^2 \rangle +$$

$$(3n_1 - 6n_2 + n_3 + n_4)\langle S_1 S_2^2 S_3^2 \rangle + (-r_0 + 3r_1 - 3r_2 - 3r_3 + 3r_4 + r_5)\langle S_1^2 S_2^2 S_3^2 \rangle,$$

$$\left\langle S_1 S_2 S_0^2 \right\rangle = 3n_1\langle S_1 S_2^2 \rangle + (r_0 - 3r_1 + 3r_2 + 3r_3)\langle S_1 S_2 \rangle + (3n_1 - 6n_2 + n_3 + n_4)\langle S_1 S_2^2 S_3^2 \rangle +$$

$$(-r_0 + 3r_1 - 3r_2 - 3r_3 + 3r_4 + r_5)\langle S_1 S_2 S_3^2 \rangle,$$

$$\left\langle S_1 S_2^2 S_0^2 \right\rangle = 3n_1\langle S_1 S_2 \rangle + (r_0 - 3r_1 + 3r_2 + 3r_3)\langle S_1 S_2^2 \rangle + (3n_1 - 6n_2 + n_3 + n_4)\langle S_1 S_2 S_3^2 \rangle,$$

$$(-r_0 + 3r_1 - 3r_2 - 3r_3 + 3r_4 + r_5)\langle S_1 S_2^2 S_3^2 \rangle,$$

$$\left\langle S_1^2 S_2^2 S_0^2 \right\rangle = 3n_1\langle S_1 S_2^2 \rangle + (r_0 - 3r_1 + 3r_2 + 3r_3)\langle S_1^2 S_2^2 \rangle + (3n_1 - 6n_2 + n_3 + n_4)\langle S_1 S_2^2 S_3^2 \rangle,$$

$$(-r_0 + 3r_1 - 3r_2 - 3r_3 + 3r_4 + r_5)\langle S_1^2 S_2^2 S_3^2 \rangle. \qquad (3.2.14)$$

If (3.2.14) is written in the form of a $21 \times 21$ matrix and solved in terms of variables $x_i$ [ ( $i = 1, 2, 3, ..., 21$ ) ( *e.g.*, $x_1 = \left\langle S_0 \right\rangle$, $x_2 = \left\langle S_1 \right\rangle, ..., x_{21} = \left\langle S_1^2 S_2^2 S_0^2 \right\rangle$ ) ] of the linear equations, all of the spin correlation functions can be determined easily as a function of the temperature, the effective field, and the anisotropy crystal-field parameter, and the longitudinal magnetic field which the other studies in the literature does not include. Since the thermal average of the central spin is equal to that of its nearest-neighbor spins within the present method, the unknown parameter $A$ can be determined numerically by the relation

$$\langle S_0 \rangle = \langle S_1 \rangle, \text{ or } x_1 = x_2 \ . \qquad (3.2.15)$$

By solving (3.2.15) numerically, at fixed values of *D/J* and *h/J*, we have obtained the parameter *A*. Then, we used the numerical values of *A* to obtain the spin correlation functions $\langle S_0 \rangle$, $\langle S_1 S_0 \rangle$, $\langle S_1 S_2 S_0 \rangle$, $\langle S_0^2 \rangle$ (quadrupole moment) and $\langle S_1^2 S_0^2 \rangle$ (biquadrupole moment) and so on.

**3.3 Solutions of Spin-1/2 and Spin-1 Ising Ferromagnetic System in a Longitudinal Magnetic Field with Transverse Field**

In the Spin-S Ising system in a longitıdinal magnetic field with transverse field the Hamiltonian is

$$H = -J \sum_{<i,j>} S_i^z S_j^z - \Omega \sum_i S_i^x - h \sum_i S_i^z \qquad (3.3.1)$$

where $S_i^z$, $S_i^x$ are the components of a spin – *S* operator at site *i*, which take the values of $S = \pm\frac{1}{2}$ for spin – 1/2 and $S = \pm 1$ and $0$ for spin -1, respectively. *J* is the exchange interaction, $\Omega$ represents the transverse field, and the first summation is over all the nearest-neighbor pairs. *h* represents the longitudinal magnetic field. For spin1/2 and spin 1 the functions are calculated with this Hamiltonian from (2.2.7)

for spin-1/2

$$F_S(x,\Omega) = \frac{1}{2} \frac{(x+h)}{\sqrt{\Omega^2 + (x+h)^2}} \tanh\left(\frac{1}{2}\beta\sqrt{\Omega^2 + (x+h)^2}\right) \qquad (3.3.2)$$

$$H_S(x,\Omega) = \left[\frac{\Omega}{\sqrt{\Omega^2 + (h+x\ )^2}}\right] \tanh\left[\frac{1}{2}\beta\sqrt{\Omega^2 + (h+x)^2}\right] \qquad (3.3.3)$$

for spin-1

$$F_S(x,\Omega)=\left[\frac{(x+h)}{\sqrt{\Omega^2+(x\ +h)^2}}\right]\frac{2\ \sinh[\beta(\ \sqrt{\Omega^2+(x\ +h)^2})]}{[1+2\ \cosh[\beta\ (\sqrt{\Omega^2+(x\ +h)^2})]} \tag{3.3.4}$$

$$H_S(x,\Omega)=\left[\frac{\Omega}{\sqrt{\Omega^2+(h+x\ )^2}}\right]\ \frac{2\ \sinh[\beta(\ \sqrt{\Omega^2+(x\ +h)^2})]}{[1+2\ \cosh[\beta\ (\sqrt{\Omega^2+(x\ +h)^2})]} \tag{3.3.5}$$

$$G_S(x,\Omega)=\left[\frac{\Omega^2+(x^2+(\Omega^2+(x\ +h)^2))}{(\Omega^2+(x\ +h)^2)}\right]\frac{\cosh[\beta\ (\ \sqrt{\Omega^2+(x\ +h)^2})]}{[1+2\ \cosh[\beta\ (\sqrt{\Omega^2+(x\ +h)^2})]} \tag{3.3.6}$$

we have to solve the equation systems (3.1.9) and (3.2.14) with parameters. Then with solving the self-consistency equation (3.2.15) for fixed transverse field. We can get the temperature dependence of the magnetization and the correlations for certain a longitudinal magnetic field and transverse field.

# CHAPTER FOUR
# NUMERICAL RESULTS AND DISCUSSIONS

In this section, we shall present numerical results for the longitudinal magnetization, hysteresis loops, susceptibility, internal energy, and specific heat of the spin -1/2 system in a longitudinal magnetic field and spin -1 system with crystal-field in a longitudinal magnetic field, respectively on the honeycomb lattice. All of the spin correlation functions mentioned above is a function of temperature, exchange interaction, crystal-field(it is absent for spin -1/2 system) and longitudinal magnetic field and depend on the value of temperature, longitudinal magnetic field and spin. If we insert the numerical values of *A* obtained from (3.2.15) into the spin correlation function $\langle S_0 \rangle$ at selected values of *h/J* for fixed value of $\frac{D}{J}$, one can find the temperature dependence of $\langle S_0 \rangle$ (it is labeled as the longitudinal magnetization $m$ ($m_0 = m_1 = m$ )) for the spin – 1 system on the honeycomb lattice.

For the spin -1/2 system(D/J = 0 in (3.2.1)), the (3.2.14) can be reduced to the form of a $6 \times 6$ matrix. The function F(x) and the spin correlation function $\langle S_i^z \rangle$ also depends on the spin value *S*. By following the same procedure as that of spin -1 system, from the (6x6) matrix, one can find the self-consistent relation corresponding to (3.2.15) for the spin -1/2 Ising model. By solving the self-consistent relation corresponding to (3.2.15) numerically for the spin -1/2 system, we have also obtained the temperature dependence of magnetization *m* on the honeycomb lattice. The numerical results are plotted in figure 4.1(a) for the spin -1/2 system. The numbers on the curves are the values of longitudinal magnetic field. As shown in figure 4.1(a), when we select the value of *h/J* = 0, the longitudinal magnetization *m* decreases continuously in the vicinity of transition temperature and vanishes at $T = T_C$; this is the second-order transition. We clearly find that the transition temperature $k_BT/J$ = 0.4551 obtained on the honeycomb lattice for the spin -1/2 system is much closer to

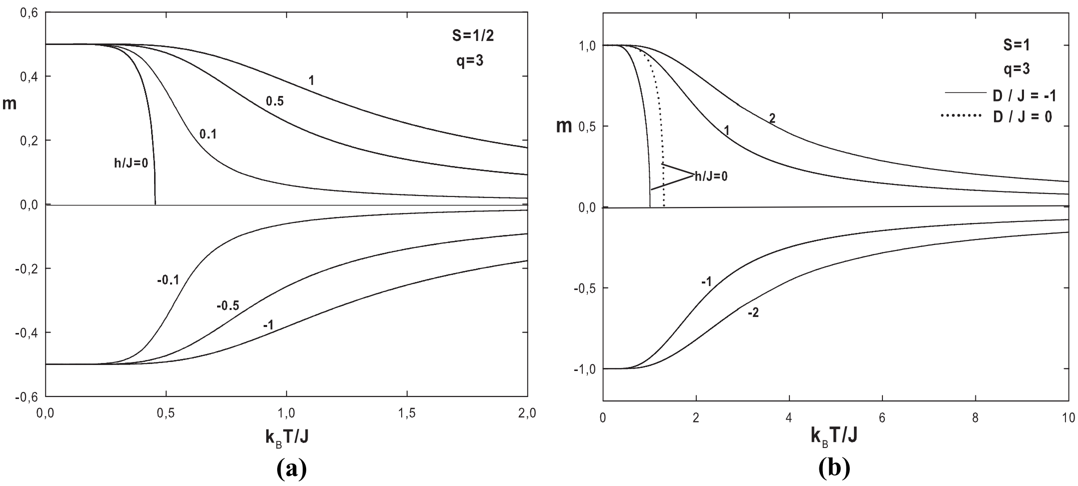



Figure 4.1 The temperature dependence of magnetizations on the honeycomb lattice: (a) for spin – 1/2 System and (b) for spin -1 system with crystal field, when the cyrstal field is selected as D/J = -1. The numbers accompanying each line are the values of the longitudinal magnetic field.

the exact value of S = 1/2 and the transition temperature value obtained on the same lattice by the expanded Bethe-Peierls approximation(EBPA) for the Ising model with S =1/2 ( Du, Liu & Yü, 2004) than those obtained by means of the equations of motion method within the Green's function(GF) formalism ( Mancini & Naddeo, 2006) and the effective field theory(EFT) ( Honmura & Kaneyoshi, 1979; Kaneyoshi et al, 1981), but it is the same with the Bethe-Peierls approximation(BPA) (Bethe, 1935; Peierls, 1936), the Bethe lattice approximation(BLA) ( Tanaka & Uryu, 1981) and the correlated effective theory(CEFT) ( Kaneyoshi & Tamura, 1982) methods found in literature.

By solving (3.2.15) numerically, for fixed value of *D/J*= -1.0 at the selected values of *h/J* = 0, 1 and 2 we have obtained the numerical values of the parameter *A*. Then, by inserting the numerical values of *A* obtained from (3.2.15) into the spin correlation function $\langle S_0 \rangle$ at selected values of *h/J* for fixed value of $\frac{D}{J}$, we have obtained the temperature dependence of magnetization($m$ = $\langle S_0 \rangle$) for the spin – 1 system on the honeycomb lattice, which are also given in figure 4.1(b). Now, we can easily find the critical temperature of the spin -1 system numerically for the fixed values of *D/J*= 0 and h/J = 0(see figure 4.1(b))

$$k_B T/J=1.3023 \tag{4.1}$$

The critical temperature value (4.1) is lower than those obtained by the various approximation methods with S =1, such as the EFT ( Kaneyoshi et al., 1981) and a new type of cluster theory(CT) in Ising models ( Kaneyoshi, 1999). But it is much closer to the transition temperature value obtained on the same lattice by the (EBPA) for the Ising model with S =1 ( Du, Liu & Yü, 2004) than those obtained by the (BLA) ( Tanaka & Uryu, 1981) and the decoupling approximation(DA) ( Kaneyoshi, 2000). For comparison, the transition temperatures $\frac{k_B T_c}{J}$ at D/J = 0 and h/J = 0 obtained by several methods and the present work for the spin -1/2 and spin -1 Ising system are given in Table 4.1

Table 4.1 Transition temperature $\frac{k_B T_c}{J}$ given at D/J = 0 and h/J = 0 by several methods and present work for honeycomb lattice with q = 3.

| S = 1/2 | | | | | | | S = 1 | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Exact | GF | EFT | DA | BLA BPA CEFT | EBPA | present work | CT | EFT | DA | BLA | EBPA | present work |
| 0.3797 | 1.82 | 0.526 | - | 0.455 | 0.420 | 0.455 | 1.428 | 1.518 | 1.398 | 1.345 | 1.284 | 1.3023 |

When we applied the longitudinal magnetic field($h$>0 or $h$<0) to the spin -1/2 and spin-1 systems, the values of magnetizations decrease slowly from their saturation magnetizations to remaining magnetizations with increasing temperatures. The remaining magnetizations become big as the longitudinal magnetic field increases. From our calculation, we can see that the longitudinal magnetization curves are symmetric for both positive and negative longitudinal magnetic field. These results are in good agreement with those of previous works (Ekiz & Keskin, 2003; Ekiz, 2005; Jiang, Bai & Wei, 2005, Jiang & Bai, 2006; Mancini & Naddeo, 2006; Wei et al, 2004), but they are quite different from those of in references (Jiang & Wei, 2000; Jiang, Wei & Xin, 2000; Jiang, Wei & Xin, 2000; Jiang et al, 2001; Htoutou et al, 2004; Polat, Akıncı & Sökmen, 2003) without applying longitudinal magnetic field.

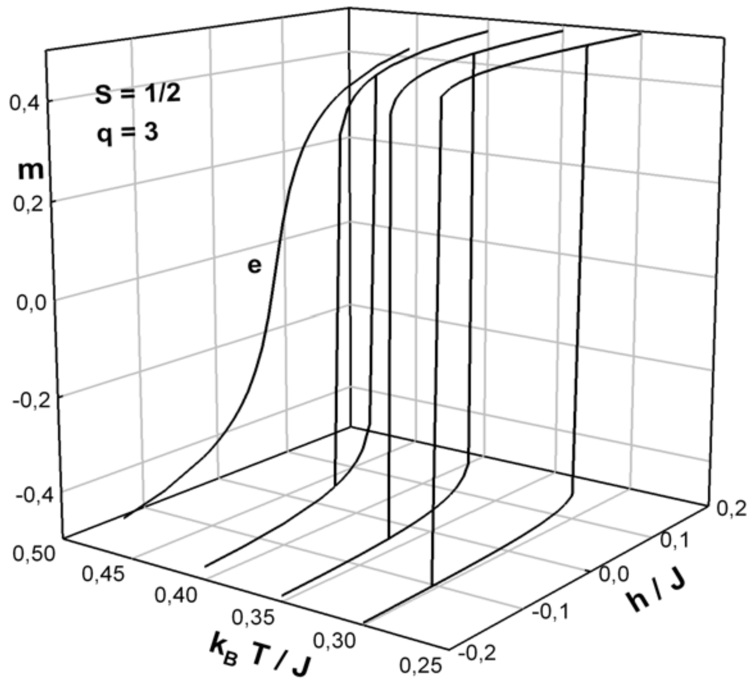
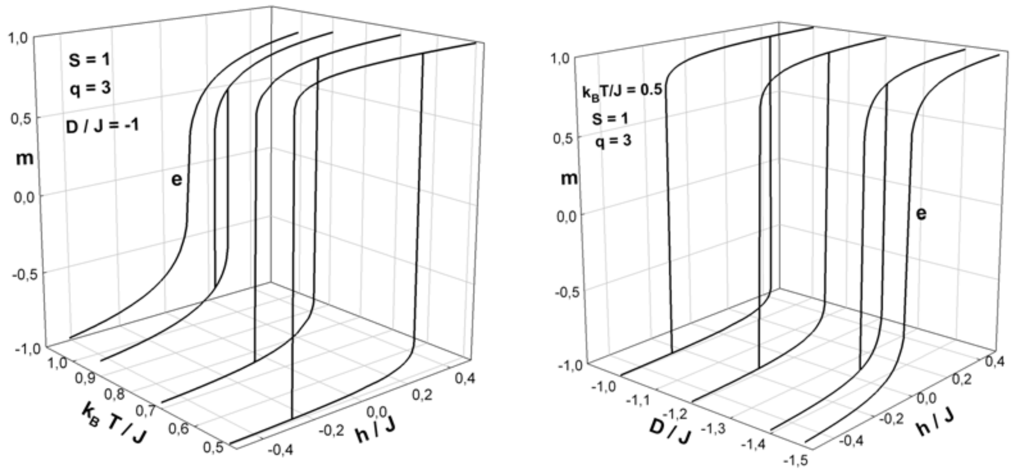



Figure 4.2 The hysteresis loops for the honeycomb lattice of spin -1/2 system in the three-dimensional space (h/J, $k_BT/J$, m ).

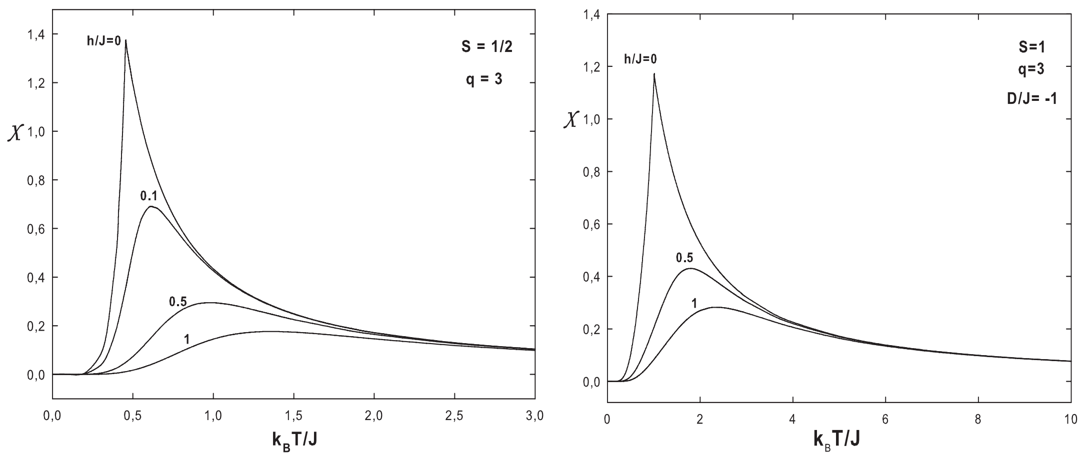
We have also investigated the influence of longitudinal magnetic field *h* on the longitudinal magnetization process at the fixed values of temperature and crystal field for the spin -1/2 system and spin -1 system with crystal field( Blume-Capel(BC) model (Balcerzak, 2003)) on the honeycomb lattice, respectively. At first, the hysteresis loops of the honeycomb lattice for spin -1/2 system in the three-dimensional space (h/J, $k_BT/J$, m ) is depicted in figure 4.2 From figure 4.2, we can see that the hysteresis loops do not occur at temperatures above the critical temperature $\frac{k_B T_c}{J} = 0.4551$, called the Curie temperature, the curve labeled *e* is such the case in figure 4.3(a). Since the coupling between nearest neighbor pair of spins is destroyed at the critical temperature, ferromagnetic system becomes paramagnetic. Moreover, the magnetic processes at low temperature which are considered to originate from the competing effects of the exchange interaction between the exchange interaction term of the nearest neighbor pair of spins and the Zeeman energy term in the Hamiltonian of the spin -1/2 system.




(a) (b)

Figure 4.3 (a) The hysteresis loops for the honeycomb lattice of spin -1system in the three - dimensional space (h/J, $k_B$T/J, m ), when the crystal field is selected as D/J = -1. (b) The hysteresis loops for the honeycomb lattice of spin -1 system in the three - dimensional space (h/J, D/J, m ), when the temperature is selected as $\frac{k_B T_c}{J}$ = 0.5.

At the fixed value of D/J = -1, the hysteresis loops of the honeycomb lattice for spin-1 system in the three-dimensional space (h/J, $k_B$T/J, m ) are plotted in figure 4.3(a). As we can see from the figures, the type of hysteresis loops become narrower with increasing temperature below the transition temperatue. Then the hysteresis loop disappears when the temperature is higher than the transition temperature as in reference (Jiang, Bai & Wei, 2005; Jiang & Bai, 2005; Jiang & Bai, 2006). When the temperature is fixed value as $\frac{k_B T}{J}$ = 0.5, the hysteresis loops for the honeycomb lattice of spin -1 system in the three-dimensional space (h/J, D/J, m ) are plotted as shown in figure 4.3(b). The type of hysteresis loops become narrower with increasing the absolute value of the crystal field. Then the hysteresis loop disappears when the absolute value of the crystal-field is large enough, the curves labeled *e* is such the case in figure 4.2 and 4.3(a). Namely, these results also show that the hysteresis loops at low temperature which are considered to originate from the competing effects of the exchange interaction between the exchange interaction term of the nearest neighbor pair of spins, and the crystal field anisotropy, and the Zeeman energy term in (3.2.1) of spin -1 system.




**(a)** **(b)**

Figure 4.4 The numerical results of the susceptibility of the spin-S system on the honeycomb lattice in the ($\chi, \dfrac{k_B T_c}{J}$) plane at the selected values of h/J = 0, 0.1, 0.5 and 1: (a) for spin – 1/2 system (b) for spin -1 system when the crystal-field is selected as D/J = -1.

Now, we state to calculate the thermodynamic parameters like susceptibility, internal energy and specific heat for the cases of spin -1/2 and spin -1 with crystal field in a longitudinal magnetic field, respectively on the honeycomb lattice. The longitudinal susceptibility for the system can be determined from the relation

$$\chi = \frac{\partial \langle S_0 \rangle}{\partial h} \tag{4.2}$$

The internal energy *U* per site of the system can be obtained easily from the thermal average of the Hamiltonian in (3.2.1). Thus, the internal energy is given by

$$-\frac{U}{NJ} = q < S_0 S_1 > + \frac{D}{J} < S_0^2 > + \frac{h}{J} \langle S_0 \rangle \tag{4.3}$$

where the correlation functions $\langle S_0 \rangle$, $\langle S_0^2 \rangle$ and $\langle S_1 S_0 \rangle$ are obtained easily from, the (3.2.14) for spin -1 system and the relation corresponding to (3.2.14) for the spin -1/2 system, respectively. With the use of (4.3), the specific heat of the system can be determined from the relation

$$C_h = \left( \frac{\partial U}{\partial T} \right)_h \tag{4.4}$$

In order to illustrate the theoretical results numerically, we have performed method calculations for the spin -1/2 and spin -1 systems on the honeycomb lattice. Thermodynamic quantities are plotted in figures 4.3 – 4.7 as a function of dimensionless temperature $\frac{k_B T}{J}$.

In figure 4.4(a), we have given the numerical results of the susceptibility for the spin – 1/2 system on the honeycomb lattice in the $(\chi, \frac{k_B T}{J})$ plane for the selected values of h/J= 0, 0.1, 0.5 and 1. We have also plotted the curves of susceptibility when the crystal-field is selected as $\frac{D}{J} = -1$ for spin -1 system in figure 4.4(b). Our results are in good agreement with those of previous works (Du, Liu & Yü, 2004; Jiang, Bai & Wei, 2005; Jiang & Bai, 2005; Jiang & Bai, 2006; Mancini & Naddeo, 2006; Wei et al, 2004). As is seen from the figures, in absence of the longitudinal magnetic field( h/J = 0), the curves of susceptibility rapidly increase and express the peak at the phase transition temperature and then rapidly decrease with the increasing temperature. In the presence of a longitudinal magnetic field the phase transition has been removed, and the stronger the longitudinal magnetic field, the smaller is the susceptibility, reflecting the fact that the longitudinal magnetization is weaker.

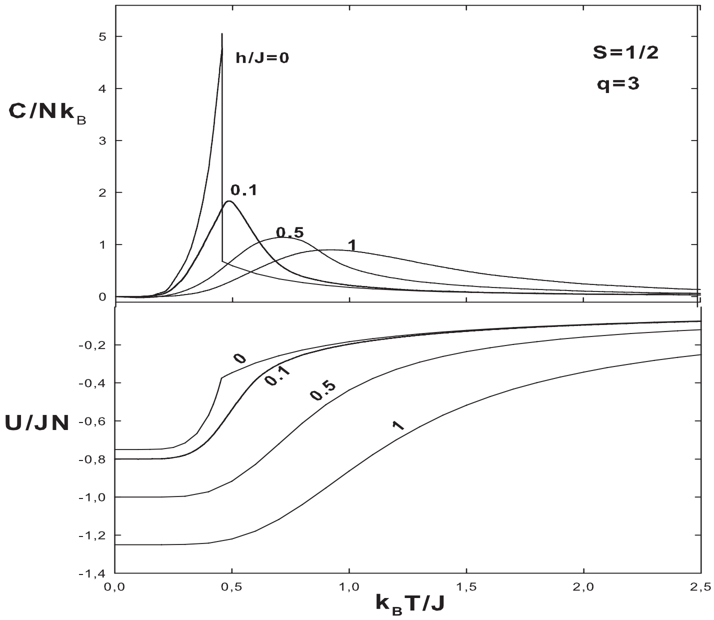
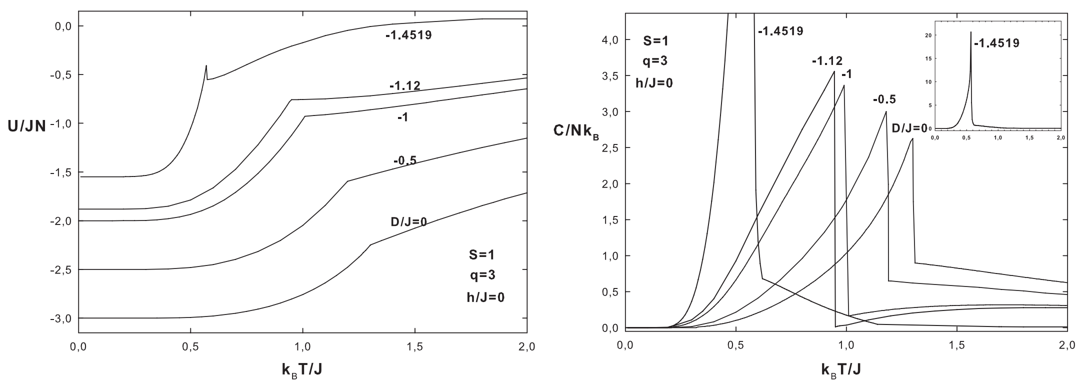



Figure 4.5 The temperature dependence of the internal energy *U* and specific heat C for the spin - 1/2 Ising model on the honeycomb lattice at selected values of *h/J* = 0, 0.1 0.5 and 1.

Finally in figures 4.5, 4.6(a-b) and 4.7(a-b), there are plotted the temperature dependences of the internal energy *U* and specific heat C in the spin -1/2 and spin -1 systems, respectively. As far as we know, these quantities of the spin -1/2 system and spin -1 system with crystal-field, respectively in a constant external field have not been reported in the literature. We can see that, if the longitudinal magnetic field increases, then the absolute value of internal energy in the spin -1/2 system and spin -1 system with crystal-field for the selected four values of *D/J* increases. In the case of *h/J* = 0, the specific heat curve of spin -1/2 system(figure 4.5) exhibits second-order phase transition at the Curie temperature $k_BT/J = 0.4551$ and rapidly decreases the increasing temperature. In the case of h/J $\neq 0$, the phase transition has been also removed, we see that with the increase of the external field the derivatives of the internal energy become flatten.

Next, in the cases of *h/J* = 0 and h/J $\neq 0$, we have plotted the temperature dependences of the internal energy *U* and specific heat C for the honeycomb lattice in the spin -1 at selected fixed values of D/J. In the case of *h/J* = 0, the behavior of internal energy with temperature and crystal-field parameter is shown in figure 4.6(a) for the honeycomb lattice at fixed values of D/J = -1.4519, -1.12, -1, -0.5, and 0. The internal energy decreases suddenly at the transition temperature as the crystal field parameter D/J gets just $D_t$/J = - 1.4519 in negative direction, which is similar to that in reference (Siqueira & Fittipaldi, 1986). The tricritical point which shows from second order to first order phase transition point in the Ising system. We can interpret it as the fact that the spin -1 Ising system ( or BC model ) exhibits a first – order

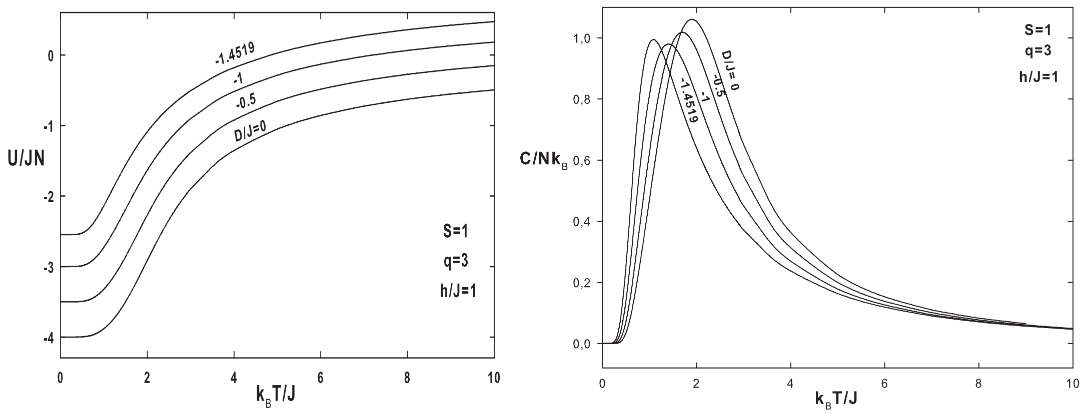



**(a)** **(b)**

Figure 4.6 The temperature dependence of (a) the internal energy *U* and (b) specific heat C for the spin-1 Ising model on the honeycomb lattice at selected fixed values of D/J = -1.4519, -1.12, - 1, -0.5 and 0, when the longitudinal magnetic field is selected as *h/J* = 0.

transition at a negative tricritical value $\frac{D_t}{J}$, such that $\frac{D_t}{J} = -1.4519$ for q = 3 ( Polat, Akıncı & Sökmen, 2003). For five selected values of the crystal-field D/J the specific heat C curves of the spin -1 system exhibit second – order phase transition at the Curie temperature. As excepted, the transition temperatures of $C/Nk_B$ increase with increasing the crystal field strenght(figure 4.6(b) ). However, when D/J becomes smaller than D/J = - 1.0, the discontinuity character of specific heat begins to increase in height. When the crystal field gets just the value of the tricritical point, a jumping in specific heat curve at the transition point appears and to increase in height (the solid curve of insert in figure 4.6(b)). This behavior could be interpreted as a competition between the exchange interaction which tries to align the spins in the same direction, and the effect of the crystal-field anisotropy which has the tendency to destroy this alignment in the considered system.

In the case of h/J $\neq 0$, our results do not have a discontinuity behavior or phase transition point at the all values of $\frac{D}{J}$ . Figure 4.7(a) curves have a continuous form and the absolute value of internal enegy for the selected four values of *D/J* increases. It is seen from figure 4.7(b) that the specific heat curves have a relatively maximum like Schottky peak at a certain value of the temperature and, in contrast to spin -1/2 system, the height of the specific heat peak for the fixed values of D/J increases and

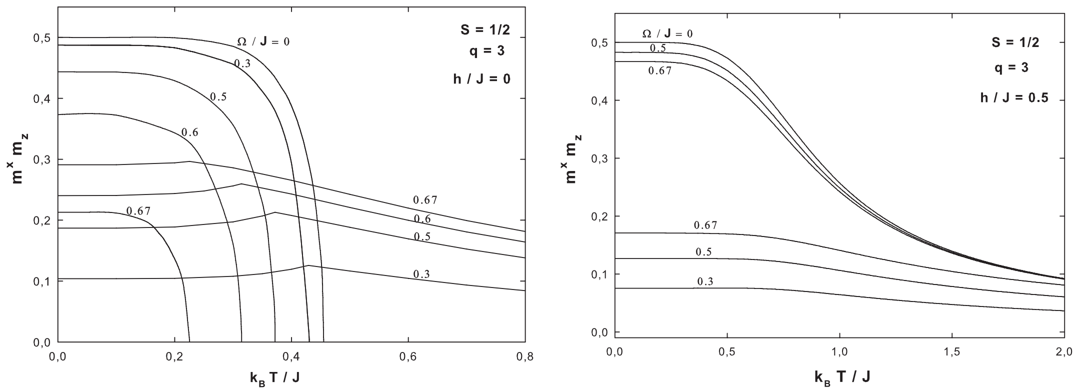



**(a)** **(b)**

Figure 4.7 The temperature dependence of (a) the internal energy *U* and (b) specific heat C for the spin –1 Ising model on the honeycomb lattice at selected five negative values of D/J = -1.4519, -1, -0.5 and 0, when the longitudinal magnetic field is selected as *h/J* = 1.

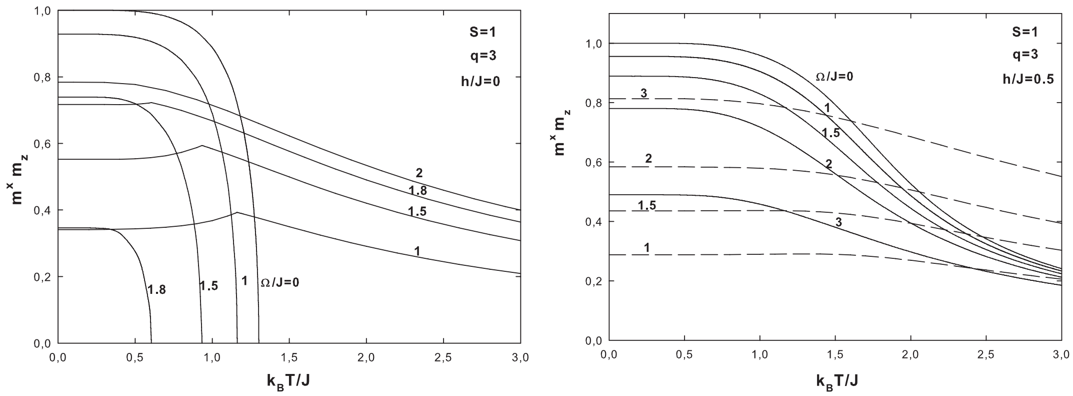
moves towards increasing temperature when the crystal-field D/J increases. We note that the Schottky-like round hump in the specific heat probably reflects the fact that the energy of system depends on the longitudinal magnetic field h/J, and the crystal field D/J. However, they do not indicate that a second-order phase transition occurs in the two dimensional system. In the case of h/J $\neq 0$, all of them may be thought as a Schottky-like peak resulting from the ferromagnetic short-range order.

The shapes of the internal energy and specific heat curves agree qualitatively with those obtained by the various methods (Blume, 1966; Capel, 1966; Du, 2003; Kaneyoshi & Jascur, 1992; Mancini & Naddeo, 2006; Micnas, 1979; Ng & Barry, 1978; Siqueira & Fittipaldi, 1986). As a result, comparing the curves for nonzero values of *h/J* we see that the phase transition has been removed in the systems. According to us, it is orginated from the presence of an external magnetic field in the




**(a)** **(b)**

Figure 4.8 Temperature dependence of the transverse magnetization $m^x$ and the longitudinal magnetization $m_z$ for the selected values of $\Omega$/J =0, 0.3, 0.5, 0.6 and 0.67 (a) when h/J = 0 for the spin -1/2 Ising ferromagnetic honeycomb lattice. (b) when h/J = 0.5 for the spin -1/2 Ising ferromagnetic honeycomb lattice.




**(a)** **(b)**

Figure 4.9 Temperature dependence of the transverse magnetization $m^x$ and the longitudinal magnetization $m_z$ for the selected values of $\Omega$/J =0, 1, 1.5, 1.8 and 2 (a) when h/J = 0 for the spin -1 Ising ferromagnetic honeycomb lattice. (b) when h/J = 0.5 for the spin -1 Ising ferromagnetic honeycomb lattice.

system. All calculated properties show the proper thermodynamical behaviour over the whole range of temperatures, including the ground state behaviour ( $\chi \to 0$ and $C \to 0$ for $T \to 0$), and the thermal stability condition ( $C_h \geq 0$ ).

By solving (3.2.15) numerically for selected fixed values of $\Omega$/J at fixed value of h/J, we have obtained the parameter $A$. Then, we used the numerical values of $A$ to obtain the spin correlation functions $< S_0^z >$ and $< S_i^x >$ numerically. They are labeled as the longitudinal magnetization $m_z$ and transverse magnetization $m^x$, respectively. At fixed value of h/J = 0., we have investigated the thermal behavior of transverse magnetization $m^x$ for the spin -1/2 Ising ferromagnetic honeycomb lattice with the corresponding selected values of Ω/J = 0.3, 0.5, 0.6 and 0.67. Our results are shown in figure 4.8(a) focusing attention to the behavior of the transverse magnetization, we can see clearly an interesting behavior. The transverse magnetization curves can be separated into two regions: the first is the nonmagnetic region in which $m_z = 0$, that is, in the ordered phase $m^x$ weakly depends on temperature, and the second is the magnetic region in which $m_z \neq 0$. The role of the transverse field Ω/J is essentially to inhibit the ordering of $m_z$ components. The thermal behavior of longitudinal and transverse magnetizations for the spin -1 Ising ferromagnetic honeycomb lattice are presented in figure 4.9(a). The results clearly show that the larger transverse field, the smaller the longitudinal magnetization $m_z$; in contrast to the longitudinal magnetization $m_z$, the transverse magnetization $m^x$ increases even at $k_BT/J = 0$, upon increasing the value of Ω/J. As is seen from figure 4.8(a) and figure 4.9(a), the saturation value of $m_z$ at $k_BT/J = 0$ decreases, when the value of Ω/J inreases. The decrease of the saturation value of $m_z$ at $k_BT/J = 0$ is closely related to the increase of the saturation value of $m^x$ at $k_BT/J = 0$ on increasing the value of Ω/J. As a result, In figure 4.8(b) and figure 4.9 (b) comparing the curves for nonzero values of *Ω/J* at the fixed value of h/J=0.5 we see that with the increase of the transverse field the longitudinal magnetization and transverse magnetization curves, respectively become flatten. Namely, the longitudinal and transverse magnetizations results of both systems exhibit similar behavior. Finally, in the present longitudinal and transverse magnetizations results are good agreement quantitatively and qualitatively with those of the effective field theory in references. (Fittipaldi, Sarmento & Kaneyoshi, 1991; Jiang & Wei, 2000).

Finally, in figure 4.10 and figure 4.11 there are plotted the temperature dependences of the internal energy(*U*) and specific heat( C ) for the spin -1/2 and spin -1 systems at selected values of transverse field and longitudinal magnetic field. We can see that, if the transverse field increases and the longitudinal magnetic field is fixed(h / J = 0.), then the absolute value of internal enegy in the systems increase

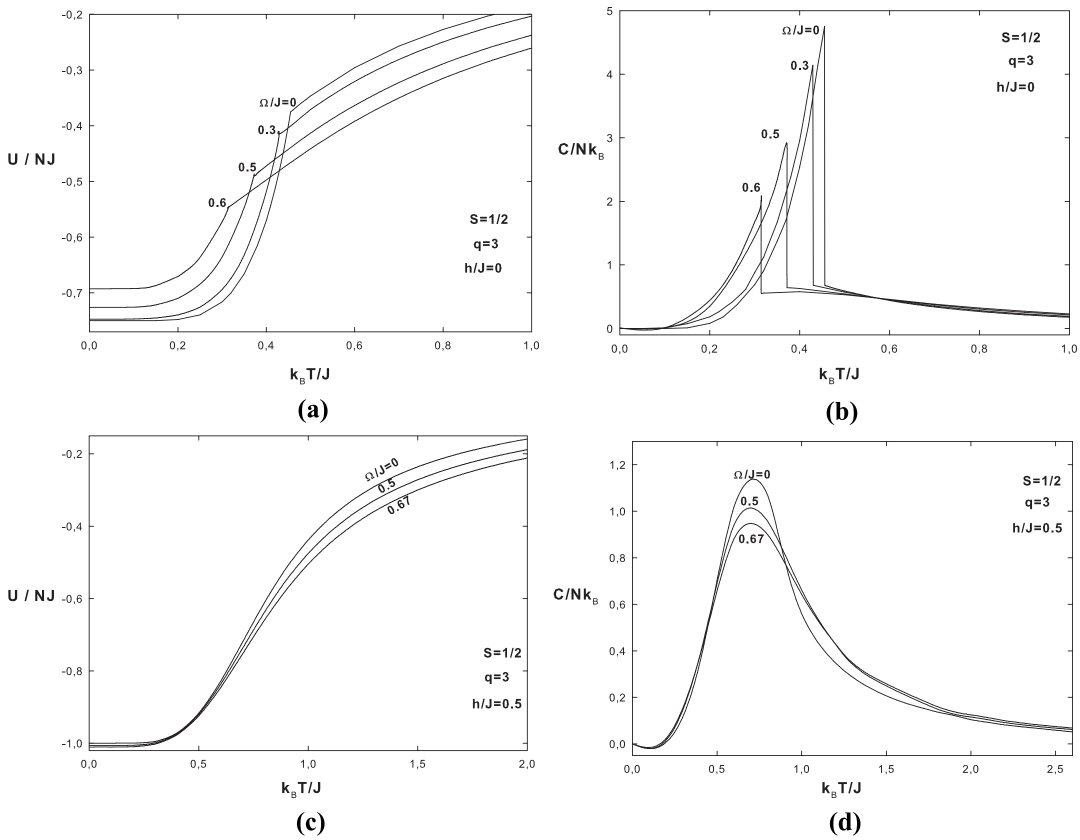



Figure 4.10 Temperature dependence of the internal energy $U$ and the specific heat $C$ for the spin -1/2 system for the selected values of $\Omega / J = 0, 0.3, 0.5, 0.6$, and $0.67$ (a) when $h / J = 0$ for internal energy $U$. (b) when $h / J = 0$ for the specific heat $C$ (c) when $h/J = 0.5$ for the internal energy $U$ (d) when $h / J = 0.5$ for the specific heat $C$

and move towards zero temperature. On the other hand, the magnetic specific heat show a cusp indicating a second-order phase change and gradually decrease in height by increasing of the transverse field strength $\Omega/J$ for the spin systems. When the strengh of the transverse field $\Omega$/J is equal to and higher than 0.67 and 1.856, respectively, all cusps in the figures disappear. As a result, comparing the curves for nonzero values of $\Omega/J$ at the fixed value of h/J we see that with the increase of the transverse field the transverse internal energy and specific heat curves, respectively become flatten. Morever, the shapes of these curves agree qualitatively with those obtained by the other approximations (Jiang & Wei, 2000; Kaneyoshi, Jascur & Fittipaldi, 1993)

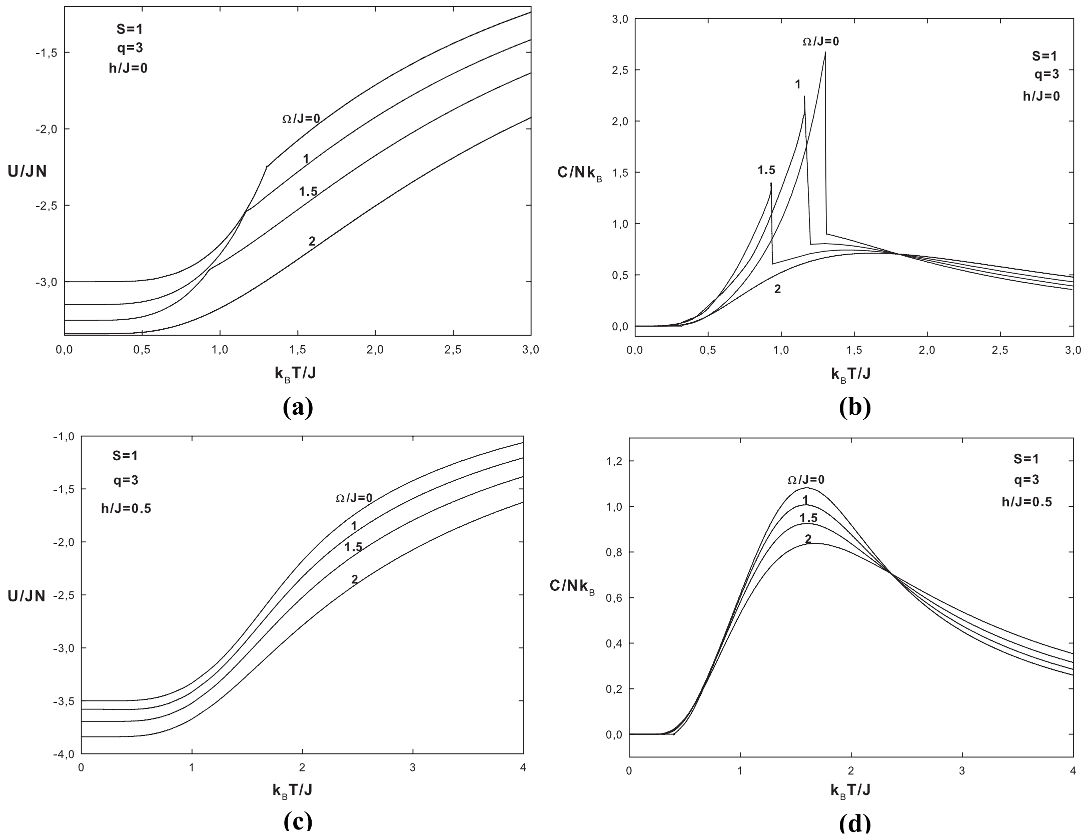



Figure 4.11 Temperature dependence of the internal energy $U$ and the specific heat $C$ for the spin -1 system for the selected values of $\Omega / J =$ 0, 1, 1.5 and 2 (a) when h / J = 0 for internal energy $U$ (b) when h / J = 0 for the specific heat $C$ (c) when h/J = 0.5 for the internal energy $U$ (d) when h / J = 0.5 for the specific heat $C$

## CHAPTER FIVE
## CONCLUSIONS

A method within the framework of the effective field theory with correlations has been proposed, which we have studied the spin -1/2 and spin -1 Ising model (or the BC model) on two dimensional honeycomb lattice. This method can be obtained easily multispin correlation functions without using a kind of decoupling approximation, so it was found that the critical temperatures of spin -1/2 system and spin -1 system with coordination number q = 3 is much closer to those obtained by the other method (Du, Liu & Yü, 2004) than those obtained by the GF and EFT for spin -1/2, and the EFT, the DA, and the BLA for the spin -1, respectively. Furthermore, we have discussed in detail the influence of the longitudinal magnetic field and transverse magnetic field on the magnetizations, susceptibilities, internal energies and specific heats of the considered systems. A number of interesting phenomena, originating from the external field have been found. The hysteresis loops and thermodynamic quantities like susceptibilitiy, internal energy and specific heat per spin can be varied depending on the temperature and value of spin.

In the previous sections we have shown and discussed some typical results for spin – 1/2 and spin -1 systems on the honeycomb lattice. On the basis of our analysis, we can conclude that the effects of the longitudinal magnetic field and the temperature in the lower-spin Ising systems are very similar to those of the higher-spin systems such as spin -3/2 and spin -2 cases ( Jiang, Bai & Wei, 2005; Jiang & Bai, 2005; Jiang & Bai, 2006; Wei et al, 2004).

In additional we discuss the temperature dependence of the longitudinal and transverse magnetizations, internal energy and specific heat for some selected value of the transverse field $\Omega / J$ for honeycomb lattice. The thermal behavior of longitudinal and transverse magnetizations for the spin -1/2 and spin -1 Ising ferromagnetic honeycomb lattice show that the larger transverse field, the smaller the longitudinal magnetization $m_z$; in contrast to the longitudinal magnetization $m_z$, the transverse magnetization $m^x$ increases even at $k_BT/J = 0$, upon increasing the value of $\Omega/J$. As a result, , in the present longitudinal and transverse magnetizations results are good agreement quantitatively and qualitatively with those of the effective field theory in references (Fittipaldi, Sarmento & Kaneyoshi, 1991; Jiang & Wei, 2000). If the transverse field increases and the longitudinal magnetic field is fixed(h/J = 0.), then the absolute value of internal energy in the systems increase and move towards zero temperature. As a result, comparing the curves for nonzero values of $\Omega/J$ at the fixed value of h/J we see that with the increase of the transverse field the transverse internal energy and specific heat curves, respectively become flatten. Morever, the shapes of these curves agree qualitatively with those obtained by the other approximations (Jiang & Wei, 2000; Kaneyoshi, Jascur & Fittipaldi, 1993)

Moreover, it could be concluded that the present method considered partially the spin-spin correlations, and has been successfully applied to a kind of spin Ising problems, which is superior to conventional mean field theory and the EFT theory in literature. Owing to the mathematical simplicity and versatility of our formulation, we hope that this new method will be potentially very useful for studying and understanding more complicated Ising ferromagnetic systems in the presence of the crystal field, transverse field and longitudinal magnetic field.

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