PHASE DIAGRAMS OF THE SPIN-1/2 ISING SYSTEMS ON TWO DIMENSIONAL LATTICES

A Thesis Submitted to the
Graduate School of Natural and Applied Sciences of
Dokuz Eylül University
In Partial Fulfilment of the Requirements for
the Degree of Master of Sciences in Physics

T.C. YÜKSEKÖĞRETİM KURULU
DOKÜMANTASYON MERKEZİ

by
Ümit Akıncı

119558

July, 2002
İZMİR

M. Sc. THESIS EXAMINATION RESULT FORM

We certify that we have read the thesis, entitled "PHASE DIAGRAMS OF THE SPIN-1/2 ISING SYSTEMS ON TWO DIMENSIONAL LATTICES" completed by ÜMİT AKINCI under supervision of DOÇ. DR. HAMZA POLAT and that in our opinion it is fully adequate, in scope and in quality, as a thesis for the degree of Master of Science.

Doç. Dr. Hamza Polat
Supervisor

119598

Prof. Dr. İsmail Sökmen
Committee Member

Prof. Dr. Doğan Demirhan
Committee Member

Approved by the
Graduate School of Natural and Applied Sciences

Prof. Dr. Cahit Helvacı
Director

ACKNOWLEDGEMENTS

I wish to express my sincere gratitude to my supervisor Assoc. Prof. Dr. Hamza Polat for his continual presence, invaluable guidance and endless patience throughout the course of this work. Also I would like to thank to Prof. İsmail Sökmen for his invaluable guidance.

I also would like to thank to Hakan Akmaz for his support about some solution techniques in Maple and his help on writing in LaTeX

I am also grateful to my father, mother and sister for their endless confidence to me throughout my life. And last I would like to thank to all my friends, without them I can't live this amazing life.

Ümit AKINCI

T.C. YÜKSEKÖĞRETİM KURULU
DOKÜMANTASYON MERKEZİ

ABSTRACT

In this work, we have studied the Kaneyoshi's differential operator technique in spin-1/2 Ising systems, i. e., the effective field theory (EFT) with correlations on honeycomb, square and triangular lattices in which attention is focused on a cluster comprising a central spin, labeled 0, and the z nearest-neighbor spins with which it directly interacts. With the use of differential operator technique and Ising spin identity, a new simple method is developed, by deriving a set of linear equations for the spin-1/2 Ising systems with three coordination numbers z ($z = 3, 4, 6$) at calculating without the decoupling approximation of the canonical ensemble averages $< s_i >, < s_i s_j >, < s_i s_j s_k >$ and $< s_i s_j ... s_z >$. By solving numerically the set of linear equations derived individually for the Ising systems, we have obtained the one, two and higher spin correlation functions as a function of temperature. The anti-Curie point has not been observed in our systems. Furthermore we have determined the phase diagrams of the spin-1/2 transverse Ising systems plotted in the $(\frac{kT}{J}, \frac{\Omega}{J})$ space. The obtained critical values of $\frac{kT}{J}$ and $\frac{\Omega}{J}$ are in good agreement with the theoretical studies in the literature.

ÖZET

Bu tezde Kaneyoshi'nin diferansiyel operatör tekniği (korelasyonlu efektif alan teorisi) spin-1/2 sistemler için, merkezi spin (0) ve etkileştiği z en yakın komşu spinden oluşan küme göz önüne alınarak balpeteği, kare ve üçgen örgülere uygulandı. Diferansiyel operatör tekniği ve Ising spin özdeşliği kullanılarak geliştirilen yeni yöntemle spin-1/2 sistemler için $< s_i >, < s_i s_j >, < s_i s_j s_k > \ldots < s_i s_j \ldots s_z >$ ortalamalarını veren denklem sistemi decoupling yaklaşımı kullanılmadan elde edildi. Bu denklem sistemi çözülerek birli, ikili ve daha yüksek korelasyon fonksiyonlarısıcaklığın fonksiyonu olarak elde edildi. Yapılan çözümler sonucu sistemlerde anti-Curie noktasına rastlanmadı. Bundan başka spin-1/2 transverse Ising sistemlerinin faz diyagramları$(\frac{kT}{J}, \frac{\Omega}{J})$ uzayında çizildi. Elde edilen kritik değerlerin $\frac{kT}{J}$ ve $\frac{\Omega}{J}$ literatürdeki değerlerle uyum içinde olduğu görüldü.

CONTENTS

Chapter One

INTRODUCTION

Chapter Two

DIFFERENTIAL OPERATOR TECHNIQUE

Chapter Three

SOLUTIONS WITHOUT DECOUPLING APPROXIMATION

T.C. YÜKSEKÖĞRETİM KURULU
DOKÜMANTASYON MERKEZİ

Chapter Four
CONCLUSIONS

LIST OF FIGURES

T.C. YÜKSEKÖĞRETİM KURULU
DOKÜMANTASYON MERKEZİ

CHAPTER ONE
INTRODUCTION

The phase transition (critical phenomena) literature is replete with models : Ising model, Heisenberg model, Potts model, Baxter model, F model, non-linear sigma model, etc. The concept of model means that systems for which it is possible (perhaps only in some limit or some dimension) to compute the partition function exactly and that is the goal of the statistical mechanics. We specify the system of interest as some sample region Ω, in which is defined the Hamiltonian H_{Ω}. The volume of the region is denoted as $V(\Omega)$ and the surface of the region (which covers the region) is denoted as $S(\Omega)$. Usually there will be boundary conditions specified on the boundary of Ω. The system may exist as a continuum (e.g. fluid) or on a lattice (e.g. magnet).

The Hamiltonian for the system can be written in a general form as follows;

$$H_{\Omega} = -\sum_{n} K_n \Theta_n \tag{1.0.1}$$

where K_n are the coupling constants and the Θ_n are the degrees of freedom (or combinations of them) which are summed in the partition function. Coupling constants are external parameters such as fields, exchange interaction parameters, temperature... For example for Zeeman effect the coupling constant is external field and corresponding degree of freedom is the magnetic moment at a lattice site.

The partition function is given by

$$Z[\{K_n\}] = Tre^{-\beta H_{\Omega}} \tag{1.0.2}$$

where $\beta = 1/k_BT$ (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. After performing this operation Z depends only the coupling constants.

The free energy is defined by

$$F_\Omega[K_n] = -k_BTlogZ_\Omega \tag{1.0.3}$$

All information about the thermodynamics of the system can be extracted from the free energy and its derivatives with respect to the coupling constants.

1.1 Thermodynamic limit

We know that from experiments, free energy is extensive for a large system, thus for a finite system we can write that

$$F_\Omega = V(\Omega)f_b + S(\Omega)f_s + O(L^{d-2}) \tag{1.1.1}$$

where f_b is the bulk free energy per unit volume (bulk free energy density) and f_s is the surface free energy per unit area, L is the characteristic linear dimension of the system and d is the dimensionality of the system. The definitions are as follows

$$\begin{aligned} f_b[\{K_n\}] &\equiv \lim_{V(\Omega)\to\infty} \tfrac{F_\Omega[\{K_n\}]}{V(\Omega)} \\ f_b[\{K_n\}] &\equiv \lim_{N(\Omega)\to\infty} \tfrac{F_\Omega[\{K_n\}]}{N(\Omega)} \\ f_s[\{K_n\}] &\equiv \lim_{S(\Omega)\to\infty} \left(\tfrac{F_\Omega[\{K_n\}]-V(\Omega)f_b[\{K_n\}]}{S(\Omega)}\right) \end{aligned} \tag{1.1.2}$$

when the limits exist and independent of Ω. (The second is about the lattice systems and there $N(\Omega)$ is number of the lattice sites in the system). The limit in these equations are known as thermodynamic limit. Some interesting notes about the history of the thermodynamic limit can be found in Dresden, 1988

T.C. YÜKSEKÖĞRETİM KURULU
DOKÜMANTASYON MERKEZİ

The axes of the phase diagram are coupling constants (e.g. pressure, temperature). In the phase diagram, regions of analiticity of $f_b[\{K_n\}]$ are called phases. The possible non-analyticities of $f_b[\{K_n\}]$ are as follows

1. $\frac{\partial f_b}{\partial K_i}$ is discontinuous. Then the transition is said to be first order phase transition.
2. $\frac{\partial f_b}{\partial K_i}$ is continuous but $\frac{\partial^2 f_b}{\partial^2 K_i}$ is discontinuous. Then the transition is said to be continuous phase transition or second order phase transition.

1.2 S-1/2 Ising model

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

$$H = -\sum_i H_i s_i - \sum_{ij} J_{ij} s_i s_j - \sum_{ijk} K_{ijk} s_i s_j s_k - \ldots \qquad (1.2.1)$$

where s_i is the spin operator at a site i, H_i is the magnetic field at a site i and J_{ij}, $K_{ijk}, \ldots$ are exchange interactions which couple two, three... spins. If one neglects the three and higher spin interactions the model is named as nearest neighbor Ising model, if one neglects the four and higher spin interactions the model is named as next nearest Ising model etc.

Ising proposed his model in 1925 and solved it for a one dimensional system(Ising, 1925). (He did not find any phase transition in one dimension. After then the physicists say that 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 representations 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 wrote 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 relationas a reccurrence relation (Baxter & Enting, 1964). Recently in 2000 Lou and Wu wrote the transfer matrices of the three dimensional Ising lattice in zero external field but they could not evaluate it (Lou & Wu, 2000), and in 2000 Istrail showed that the three dimensional Ising model cannot be solved analytically (Istrail, 2000). Until now physicists have not reached the exact solution of the two dimensional Ising model with external field and three dimensional Ising model.

Besides 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 an 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 demonstrated that at a sufficiently low temperatures the Ising model in two or three dimensions must exhibit a phase transition (Peierls, 1936) .

1.3 Analytic and symmetry properties of the Ising model

The nearest neighbor Ising model's Hamiltonian is

$$H = -J\sum_{ij} s_i s_j - H\sum_{i} s_i \tag{1.3.1}$$

The magnetization per site is given by

$$M = -\frac{1}{N}\frac{\partial F}{\partial H} \tag{1.3.2}$$

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 $S = -\partial f/\partial T \geq 0$
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 imply that specific heat at constant magnetic field and the isothermal susceptibility are greater than (or equal to) zero.

$$\begin{aligned} C_H &= -T\tfrac{\partial^2 f}{\partial T^2}|_H \geq 0 \\ \chi_T &= -\tfrac{\partial^2 f}{\partial H^2}|_T \geq 0 \end{aligned} \tag{1.3.3}$$

Proofs of the properties can be found in Goldenfeld, 1992

By inspection one can show that

$$\sum_{\{s_i=\pm1\}} \phi(\{s_i\}) = \sum_{\{s_i=\pm1\}} \phi(\{-s_i\}) \tag{1.3.4}$$

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

1. Time-reversal symmetry :

   (1.3.1) implies that

$$H(H, J, \{s_i\}) = H(-H, J, \{-s_i\}) \tag{1.3.5}$$

T.C. YÜKSEKÖĞRETİM KURULU
TASYON MERKEZİ

by using (1.0.2) in (1.0.3) and with (1.3.5) one can show that

$$f(H,J,T) = f(-H,J,T) \tag{1.3.6}$$

e.g. the free energy is even in H.

2. Sub-lattice 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 such that s_i^A are interact only with s_i^B (and vice versa).Under no magnetic field one can show that

   $$H(0,-J,\{s_i^A\},\{s_i^B\}) = H(0,J,\{s_i^A\},\{-s_i^B\}) \tag{1.3.7}$$

   and it can be shown that this implies

   $$f(0,J,T) = f(0,-J,T) \tag{1.3.8}$$

   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

1.4 Importance of thermodynamic limit and spontaneous symmetry breaking

Magnetization is given by

$$M = -\frac{1}{N}\frac{\partial F(H)}{\partial H} \tag{1.4.1}$$

From the time reversal symmetry ($F(H,J,T) = F(-H,J,T)$)

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

Thus

$$M(H) = -M(-H) \qquad (1.4.2)$$

At $H = 0$ we must have

$$M(0) = -M(0) = 0 \qquad (1.4.3)$$

This shows that the magnetization in zero external field must be zero!

But this is true only for finite systems. It fails in the thermodynamic limit, because $F(H)$ can develope a discontinuity in its first derivative $\partial F(H)/\partial H$. Indeed (1.3.7) does not imply (1.4.4) unless one makes 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 :

$$F(H) = F(0) + O(H^n) \qquad (1.4.4)$$

where $n > 1$ and

$$\lim_{\epsilon\to 0} \frac{f(+\epsilon) - f(0)}{\epsilon} = \lim_{\epsilon\to 0} \frac{f(-\epsilon) - f(0)}{\epsilon} = 0 \qquad (1.4.5)$$

However none of the properties of $f(H)$ guarantee that smoothness. Instead of (1.4.5) one can write $f(H)$ as follows :

$$F(H) = F(0) - M_s\,|H| + O(H^n) \qquad (1.4.6)$$

where $n > 1$. (1.4.6) 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

$$\begin{aligned} M_s &= \lim_{H\to 0^+} -\frac{\partial f(H)}{\partial H} \\ -M_s &= \lim_{H\to 0^-} -\frac{\partial f(H)}{\partial H} \end{aligned} \qquad (1.4.7)$$

M_s is a function of temperature. At zero temperature M_s should be unity. As the temperature rises towards 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 are known as spontaneous symmetry breaking. T_c is known as the critical point (Curie temperature).

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 ferroelectric systems the order parameter is electric polarization, for superfluid systems condensate wave function and the superconductors ground state wave function.

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

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

$$\lambda = \lim_{t \to 0} \frac{\ln |F(t)|}{\ln |t|} \tag{1.5.1}$$

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

$$F(t) \sim |t|^{\lambda} \tag{1.5.2}$$

(1.5.2) explains the behaviour of the thermodynamic function $F(t)$ near the critical point (T_c).

Another important concept is universality, it classifies the systems with three parameters : 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 this details.

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

1.6 Extensions 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 to 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 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 a combination of a lattice gas and the spin model. Here each site can have three values $s_i = 0, \pm 1$. This model was first used to model liquid $^3He -^4 He$ mixtures. In the q-state Potts model (Potts, 1952) each site has one of the q values, and the interaction between two neighboring sites is $-J$ if the two sites have the same value; otherwise the interaction is zero.

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.

CHAPTER TWO
DIFFERENTIAL OPERATOR TECHNIQUE

2.1 Callen identity

The Hamiltonian of the S-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 z component of the spin operator 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

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

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

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 (2.1.1).For this purpose , the Hamiltonian is separated into two parts (which are commute with each other). One part is about the i th site and the other part does not depend on the site i.

$$H = H_i + H' \tag{2.1.4}$$

with

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

T.C. YÜKSEKÖĞRETİM KURULU
'ON MERKEZİ

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 parts are commute with each other (because $[s_i, s_j] = 0$ 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

$$\begin{aligned} < s_i > &= \frac{1}{Z}\left\{Tre^{-\beta H}\tanh(\beta E_i)\right\} \\ &= < \tanh(\beta E_i) > \end{aligned} \tag{2.1.8}$$

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

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

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

$$< \{f_i\}\, s_i^z > = S < \{f_i\}\, B_S(\beta E_i) > \tag{2.1.10}$$

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 is 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 ($s_i = \pm 1$) (Matsudai, 1973)

$$\begin{aligned} \tanh(Ks_1) &= As_1, & A &= \tanh(K) \\ \tanh(Ks_1 + Ks_2) &= B(s_1 + s_1), & B &= \tfrac{1}{2}\tanh(2K) \\ \tanh(Ks_1 + Ks_2 + Ks_3) &= C_1(s_1 + s_2 + s_3) + C_2(s_1 s_2 s_3), && \\ & \quad C_1 = \tfrac{1}{4}(\tanh(3K) + \tanh(K)), && \\ & \quad C_2 = \tfrac{1}{4}(\tanh(3K) - \tanh(K)) && \end{aligned} \tag{2.1.12}$$

Similar relations can be expressed for higher number of spins. (But it is rather difficult 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 operates on the function of x and it gives;

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

where a is a constant, $\nabla = \partial/\partial x$ is the differential operator and $f(x)$ is an arbitrary function of x. This can be seen with expanding the exponential term in a 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 by using (2.2.1)

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

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

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

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

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

In general (2.2.4) and (2.2.5) can be written as

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

(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);

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

where λ_n are the eigenvalues of $-H_i$ and φ_n are their corresponding eigenvectors. H_i is the Hamiltonian of 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 one 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 acting on the system.

Average magnetizations, critical temperatures, internal energies, susceptibilities and specific heats can be computed with the differential operator technique and then one can gain the phase diagrams of the different systems. (2.2.6) is an exact relation for the Ising system but for evaluating (2.2.6) one needs to make some approximations, then it gives an approximate solutions for the system. With these approximations, (2.2.6) can give MFA and Zernike approximation's results. (Kaneyoshi, 1993). Besides this, from (2.2.6) one can gain the results which are 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 is difficult, it is rather simple to apply differential operator technique to higher spin Ising systems. (2.2.6) can evaluate with the expansion of 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 by using Van der Waerden identity respectively (a is an arbitrary constant)

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

and for higher spin Ising systems these identities become more complex and one needs 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_δ) in the system and form a cluster. From (2.2.6) we get for the central spin in the cluster

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

and for the perimeter spin in the cluster

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

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 any function of the spin variable except s_δ and $\{f_0\}$ is any function of the spin variable except s_0. Instead of 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 central spin and the other is the interaction of the perimeter spin with the neighbor spins outside the cluster. The latter is treated with an effective field (h)

$$E_\delta = J\sum_{j=1}^{z} s_{\delta+j} = J s_0 + J\sum_{\substack{j=1 \\ j\neq-\delta}}^{z} s_{\delta+j} = J s_0 + (z-1)h \tag{2.3.3}$$

where h is the effective field per perimeter spin.

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

$$\begin{aligned} < \{f_0\}\, s_0 > &= < \{f_0\}\, e^{J\sum_{\delta=1}^{z} s_\delta \nabla} > f(x)|_{x=0} \\ &=< \{f_0\} \prod_{\delta=1}^{z} e^{J s_\delta \nabla} > f(x)|_{x=0} \end{aligned} \tag{2.3.4}$$

$$\begin{aligned} < \{f_\delta\}\, s_\delta > &= < \{f_\delta\}\, e^{(J s_0 + (z-1)h)\nabla} > f(x)|_{x=0} \\ &=< \{f_\delta\}\, e^{J s_0 \nabla} > f(x+\alpha)|_{x=0} \end{aligned} \tag{2.3.5}$$

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

2.4 S-1/2 systems

With (2.2.8) for S-1/2 systems, (2.3.4) and (2.3.5) becomes

$$\begin{aligned} < \{f_0\}\, s_0 > &= < \{f_0\} \prod_{\delta=1}^{z} [\cosh(J\nabla) + s_\delta \sinh(J\nabla)] > f(x)|_{x=0} & (2.4.1) \\ < \{f_\delta\}\, s_\delta > &= < \{f_\delta\} [\cosh(J\nabla) + s_0 \sinh(J\nabla)] > f(x+\alpha)|_{x=0} & (2.4.2) \end{aligned}$$

With $\{f_\delta\} = 1$ and $\{f_0\} = 1$ we can get $< s_0 >$ and $< s_\delta >$ which are the average magnetizations of the central spin and the perimeter spin in our cluster.

$$\begin{aligned} < s_0 > &= < \prod_{\delta=1}^{z} [\cosh(J\nabla) + s_\delta \sinh(J\nabla)] > f(x)|_{x=0} & (2.4.3) \\ < s_\delta > &= < [\cosh(J\nabla) + s_0 \sinh(J\nabla)] > f(x+\alpha)|_{x=0} & (2.4.4) \end{aligned}$$

The average magnetizations of the perimeter spins in the cluster (s_δ) can be considered wholly equal to each other. Because their average magnetization equations (2.4.4) are the same.

$$< s_1 > = < s_2 > = < s_3 > = \ldots = < s_z > \qquad (2.4.5)$$

From (2.4.4) one can arrive the perimeter spin's average magnetization

$$\begin{aligned} < s_\delta > &= [\cosh(J\nabla)] f(x+\alpha)|_{x=0} + < s_0 > [\sinh(J\nabla)] f(x+\alpha)|_{x=0} \\ < s_\delta > &= a_1 + a_2 < s_0 > & (2.4.6) \end{aligned}$$

where

$$\begin{aligned} a_1 &= [\cosh(J\nabla)] f(x+\alpha)|_{x=0} \\ a_2 &= [\sinh(J\nabla)] f(x+\alpha)|_{x=0} & (2.4.7) \end{aligned}$$

Here $f(x)$ may vary from one S-1/2 system to other and it depends on the system as well as the fields acting on the system (magnetic field, transverse field, etc...) since one can write $\cosh(J\nabla)$ and $\sinh(J\nabla)$ in terms of the $\exp(J\nabla)$

$$\begin{aligned} \cosh(J\nabla) &= \frac{1}{2}(e^{J\nabla} + e^{J\nabla}) \\ \sinh(J\nabla) &= \frac{1}{2}(e^{J\nabla} - e^{J\nabla}) \end{aligned}$$

T.C. YÜKSEKÖGRETİM KURULU
DOKÜMANTASYON MERKEZİ

then with (2.2.1)

$$\begin{aligned} a_1 &= \tfrac{1}{2}[f(\alpha+J)+f(\alpha-J)] \\ a_2 &= \tfrac{1}{2}[f(\alpha+J)-f(\alpha-J)] \end{aligned} \tag{2.4.8}$$

One trick for evaluating (2.4.3) is the decoupling approximation. When (2.4.3) is expanded for any z, the terms like $< s_1 s_2 s_3 ... >$ can be written as

$$< s_1 s_2 s_3 ... s_z > = < s_1 >< s_2 >< s_3 > ... < s_z > \tag{2.4.9}$$

For S-1/2 Ising system $s_0^2 = s_0^4 = ... = s_0^{2n} = 1$ and from this $s_0^3 = s_0^5 = ... = s_0^{2n+1} = s_0$ where n is the positive integer.(i.e. the odd powers of the central spin operator is equal to central spin operator and the even powers of the central spin operator is equal to 1).

Since (2.4.5) is valid for all S-1/2 Ising systems with decoupling approximation (2.4.9), (2.4.3) can be written as follows

$$\begin{aligned} < s_0 > &= < [\cosh(J\nabla) + s_\delta \sinh(J\nabla)]^z > f(x)|_{x=0} \\ < s_0 > &= \binom{z}{r} < s_\delta >^r \sinh^r(J\nabla)\cosh^{z-r}(J\nabla) f(x)|_{x=0} \end{aligned} \tag{2.4.10}$$

For $z = 3, 4, 6$ central spin average magnetizations can be obtained by (2.4.10) by choosing only the odd operators in (2.4.10) (Since $f(x)$ is odd in x, only when odd operators act on it gives results different from zero)

$$< s_0 > = 3 < s_\delta > K_{31} + < s_\delta^3 > K_{32} \tag{2.4.11}$$

for $z = 3$

$$< s_0 > = 4 < s_\delta > K_{41} + 4 < s_\delta^3 > K_{42} \tag{2.4.12}$$

for $z = 4$

$$< s_0 > = 6 < s_\delta > K_{61} + 20 < s_\delta^3 > K_{62} + 6 < s_\delta^5 > K_{63} \tag{2.4.13}$$

for $z = 6$

The coefficients for $z = 3, 4, 6$

$$\begin{aligned}
K_{31} &= \sinh(J\nabla)\cosh^2(J\nabla)f(x)|_{x=0} \\
K_{32} &= \sinh^3(J\nabla)f(x)|_{x=0} \\
K_{41} &= \sinh(J\nabla)\cosh^3(J\nabla)f(x)|_{x=0} \\
K_{42} &= \sinh^3(J\nabla)\cosh(J\nabla)f(x)|_{x=0} \\
K_{61} &= \sinh(J\nabla)\cosh^5(J\nabla)f(x)|_{x=0} \\
K_{62} &= \sinh^3(J\nabla)\cosh^3(J\nabla)f(x)|_{x=0} \\
K_{63} &= \sinh^5(J\nabla)\cosh(J\nabla)f(x)|_{x=0}
\end{aligned} \tag{2.4.14}$$

With inserting (2.4.6) in the equations (2.4.11),(2.4.12) and (2.4.13) we can find the central spin average magnetizations for the honeycomb, square and triangular lattices. Then for finding the unknown effective field (h) one can use the self-consistency condition for the effective field theories

$$< s_0 >=< s_\delta > \tag{2.4.15}$$

Since we choose the central spin randomly in the system, we must use (2.4.15). After performing decoupling approximation one can find

$$\begin{aligned}
< s_\delta^3 > &= a_1^3 + 3a_1a_2^2 + < s_0 > (3a_1^2a_2 + a_2^3) \\
< s_\delta^5 > &= a_1^5 + 10a_1^3a_2^2 + 5a_1a_2^4 + < s_0 > (5a_1^4a_2 + 10a_1^2a_2^3 + a_2^5)
\end{aligned} \tag{2.4.16}$$

By using (2.4.16) in (2.4.11), (2.4.12) and (2.4.13) one can obtain the central spin average magnetizations for the $z = 3, 4, 6$

$$< s_0 >= \frac{3K_{31}a_1 + 3K_{32}a_1a_2^2 + K_{32}a_1^3}{1 - (3K_{31}a_2 + 3K_{32}a_1^2a_2 + K_{32}a_2^3)} \tag{2.4.17}$$

for $z = 3$

$$< s_0 >= \frac{4K_{41}a_1 + 12K_{42}a_1a_2^2 + 4K_{42}a_1^3}{1 - (4K_{41}a_2 + 12K_{42}a_1^2a_2 + 4K_{42}a_2^3)} \tag{2.4.18}$$

for $z = 4$

$$< s_0 >= \frac{6K_{61}a_1 + 20K_{62}a_1^3 + 60K_{62}a_1a_2^2 + 6K_{63}a_1^5 + 60K_{63}a_1^3a_2^2 + 30K_{63}a_1a_2^4}{1 - (6K_{61}a_2 + 60K_{62}a_1^2a_2 + 20K_{62}a_2^3 + 30K_{63}a_1^4a_2 + 60K_{63}a_1^2a_2^3 + 6K_{63}a_2^5)} \tag{2.4.19}$$

for $z = 6$

On the other hand from (2.4.15) and (2.4.6)

$$< s_0 >= \frac{a_1}{1 - a_2} \tag{2.4.20}$$

Thus the fundamental equations for $z = 3, 4, 6$ can be found by equating (2.4.17), (2.4.18) and (2.4.19) to (2.4.20)

$$\frac{3K_{31}a_1 + 3K_{32}a_1a_2^2 + K_{32}a_1^3}{1 - (3K_{31}a_2 + 3K_{32}a_1^2a_2 + K_{32}a_2^3)} - \frac{a_1}{1 - a_2} = 0 \tag{2.4.21}$$

for $z = 3$

$$\frac{4K_{41}a_1 + 12K_{42}a_1a_2^2 + 4K_{42}a_1^3}{1 - (4K_{41}a_2 + 12K_{42}a_1^2a_2 + 4K_{42}a_2^3)} - \frac{a_1}{1 - a_2} = 0 \tag{2.4.22}$$

for $z = 4$

$$\frac{6K_{61}a_1 + 20K_{62}a_1^3 + 60K_{62}a_1a_2^2 + 6K_{63}a_1^5 + 60K_{63}a_1^3a_2^2 + 30K_{63}a_1a_2^4}{1 - (6K_{61}a_2 + 60K_{62}a_1^2a_2 + 20K_{62}a_2^3 + 30K_{63}a_1^4a_2 + 60K_{63}a_1^2a_2^3 + 6K_{63}a_2^5)}$$
$$- \frac{a_1}{1 - a_2} = 0 \tag{2.4.23}$$

for $z = 6$.

From these equations one can obtain the dependence of the effective field to the temperature and the fields acting on the system for the $z = 3, 4, 6$ and then one can obtain magnetizations, susceptibilities, internal energies, specific heats and phase diagrams for these lattices. Also by determining the functions of the various S-1/2 Ising systems (under the external magnetic field, transverse field, etc.) from (2.2.7), one can obtain for these system's phase diagrams from (2.4.21), (2.4.22) and (2.4.23) for $z = 3, 4, 6$.

The coefficients in (2.4.21), (2.4.22), (2.4.23) can be calculated by writing $\cosh(J\nabla)$, $\sinh(J\nabla)$ and their products (which are form the odd operators in

$(J\nabla)$ in terms of the $e^{J\nabla}$ and by (2.2.1)

$$\begin{aligned} a_1 &= \tfrac{1}{2}(f(\alpha+J)+f(\alpha-J)) \\ a_2 &= \tfrac{1}{2}(f(\alpha+J)-f(\alpha-J)) \\ K_{31} &= \tfrac{1}{4}(f(3J)+f(J)) \\ K_{32} &= \tfrac{1}{4}(f(3J)-3f(J)) \\ K_{41} &= \tfrac{1}{8}(f(4J)+2f(2J)) \\ K_{42} &= \tfrac{1}{8}(f(4J)-2f(2J)) \\ K_{61} &= \tfrac{1}{32}(f(6J)+4f(4J)+5f(2J)) \\ K_{62} &= \tfrac{1}{32}(f(6J)-3f(2J)) \\ K_{63} &= \tfrac{1}{32}(f(6J)-4f(4J)+5f(2J)) \end{aligned} \tag{2.4.24}$$

In the S-1/2 Ising systems without any external field the Hamiltonian is

$$H = -J\sum_{<i,j>} s_i^z s_j^z, \qquad s_i^z = \pm 1$$

and the function is calculated with this Hamiltonian from (2.2.7)

$$f(x) = \tanh(\beta x) \tag{2.4.25}$$

In the S-1/2 Ising systems with external magnetic field the Hamiltonian is

$$H = -J\sum_{<i,j>} s_i^z s_j^z - H\sum_i s_i^z$$

and the function is calculated with this Hamiltonian from (2.2.7)

$$f(x) = \tanh(\beta x + \beta H) \tag{2.4.26}$$

In the S-1/2 Ising systems with transverse field the Hamiltonian is

$$H = -J\sum_{<i,j>} s_i^z s_j^z - \Omega\sum_i s_i^x$$

(where Ω is the transverse field) and the function is calculated with this Hamiltonian from (2.2.7)

$$f(x) = \frac{x}{\sqrt{\Omega^2 + x^2}}\tanh(\beta\sqrt{\Omega^2 + x^2}) \tag{2.4.27}$$

2.5 Thermodynamic properties

The susceptibility (under the magnetic field H) is given by;

$$\chi(T) = \frac{\partial m(T,H)}{\partial H} \qquad (2.5.1)$$

Once effective field (h) is calculated from (2.4.21) (or from (2.4.22), (2.4.23) for $z = 4$, $z = 6$) then one can obtain from (2.4.20) the magnetization then with (2.5.1) the susceptibility.

The internal energy of the system can be obtained from the thermodynamic average of the Hamiltonian

$$U = < H > \qquad (2.5.2)$$

For the systems S-1/2 with the Hamiltonian (2.1.1)

$$\frac{U}{N} = -\frac{1}{2} < E_i s_i > - H < s_i > \qquad (2.5.3)$$

where N is the total number of spins in the system. $< E_i s_i >$ for S-1/2 can be calculated from (2.4.2) with $\{f_i\} = E_i$ or it can be evaluated from this relation:

$$< E_i s_i > = \left[\frac{\partial}{\partial y} < e^{yE_i} >\right]_{\nabla = y} f(x)|_{x=0}$$

Then one can obtain this term

$$\begin{aligned} < E_i s_i > = {} & zJ(\sinh(J\nabla) + < s_0 > \cosh(J\nabla))(\cosh(J\nabla) \\ & + < s_0 > \sinh(J\nabla))^{z-1} f(x)|_{x=0} \end{aligned} \qquad (2.5.4)$$

Then, the specific heat can be calculated by using

$$C(T) = \frac{\partial U}{\partial T} \qquad (2.5.5)$$

Thus, for example with (2.4.21), (2.4.24), (2.4.26) and (2.4.20), (2.5.1), (2.5.3), (2.5.4), (2.5.5) we have a complete description of the S-1/2 Ising system with an external magnetic field (and similarly for the other systems we get the complete description of the system via suitable equations)

CHAPTER THREE
SOLUTIONS WITHOUT DECOUPLING APPROXIMATION

3.1 Method

Instead of making decoupling approximation in (2.4.3) we can expand it for certain z and evaluate the terms like $< s_1 s_2 s_3 ... s_z >$ via (2.4.2) by choosing suitable $\{f_\delta\}$ and the terms like $< s_0 s_2 s_3 ... s_{z-1} >$ via (2.4.1) by choosing suitable $\{f_0\}$. (e.g. for $< s_0 s_2 >$ the $\{f_0\} = s_2$ in (2.4.1)). In this way we can obtain the equations of all the correlations in our system. Then we can solve this system of equations and get the correlations and magnetizations as a function of temperature, external fields and effective field. Similar to the given formulation in section 2 we use here effective field concept and then (2.4.1) and (2.4.2) are our fundamental relations.

$$
\begin{aligned}
< \{f_0\}\, s_0 > \;&=\; < \{f_0\} \prod_{\delta=1}^{z} [\cosh(J\nabla) + s_\delta \sinh(J\nabla)] > f(x)|_{x=0} && (3.1.1)\\
< \{f_\delta\}\, s_\delta > \;&=\; < \{f_\delta\} \, [\cosh(J\nabla) + s_0 \sinh(J\nabla)] > f(x+\alpha)|_{x=0} && (3.1.2)
\end{aligned}
$$

with $\{f_0\} = 1$ and $\{f_\delta\} = 1$ (3.1.1) and (3.1.2) reduce to the central spin and the perimeter spin magnetization equations

$$
\begin{aligned}
< s_0 > \;&=\; < \prod_{\delta=1}^{z} [\cosh(J\nabla) + s_\delta \sinh(J\nabla)] > f(x)|_{x=0} && (3.1.3)\\
< s_\delta > \;&=\; < [\cosh(J\nabla) + s_0 \sinh(J\nabla)] > f(x+\alpha)|_{x=0} && (3.1.4)
\end{aligned}
$$

and with the effective field concept (3.1.4) reduces to

$$
< s_\delta >= a_1 + a_2 < s_0 > \qquad (3.1.5)
$$

EKÖĞRETİM KURULU
MERKEZİ

Here a_1, a_2 are given by (2.4.8). Also we can use (2.4.5) here since we use effective field concept. When we obtain the central and the perimeter spin magnetizations (by substituting the correlations in) as a function of the temperature, external fields and effective field, with (2.4.15) we can obtain the temperature dependence of the effective field (for fixed external fields). Then we can get all magnetizations and correlations as a function of the temperature and external fields acting on our system.

For obtaining critical temperature, we solve the self-consistency equation under the assumption that effective field is so small in the vicinity of the critical temperature. We set the effective field to zero or so small value in the self-consistency equation then we solve the equation under this assumption to get the critical temperature for certain external fields.

3.2 Honeycomb lattice

For the S-1/2 Ising system with $z = 3$ (honeycomb lattice) we start by expanding (3.1.3) for $z = 3$. We have to choose only odd operators in this expansion (like $\sinh(J\nabla)\cosh^2(J\nabla)$) because when even operators operate on $f(x)$ (which is odd in x) they give zero. Thus we obtain

$$< s_0 >= K_{31}(< s_1 > + < s_2 > + < s_3 >) + K_{32}(< s_1 s_2 s_3 >) \tag{3.2.1}$$

The coefficients K_{31} and K_{32} are given by (2.4.24). We know that the correlations are depended only on the distance between the spins. Then we can say that in our systems some of the correlations are equal to the other.

$$\begin{aligned} < s_0 s_1 > &= < s_0 s_2 >=< s_0 s_3 > \\ < s_1 s_2 > &= < s_1 s_3 >=< s_2 s_3 > \\ < s_0 s_1 s_2 > &= < s_0 s_1 s_3 >=< s_0 s_2 s_3 > \end{aligned} \tag{3.2.2}$$

Also from the validity of (2.4.5) in this formulation

$$< s_1 >=< s_2 >=< s_3 > \tag{3.2.3}$$

The perimeter spin - perimeter spin correlations can be obtained by (3.1.2) and the central spin -perimeter spin correlations can be obtained by (3.1.1). Also they depend on the other correlations (like central spin - perimeter spin - perimeter spin) From (3.2.1) by using $s^2 = 1$ (this is valid for all S-1/2 Ising system because $s = \pm 1$)

$$< s_0 s_1 >= K_{31}(1+ < s_1 s_2 > + < s_1 s_3 >) + K_{32} < s_2 s_3 > \tag{3.2.4}$$

and from (3.1.5)

$$< s_1 s_2 >= a_1 < s_2 > +a_2 < s_0 s_2 > \tag{3.2.5}$$

from (3.2.4) and (3.2.5)

$$\begin{aligned} < s_0 s_1 s_2 > &= K_{31}(< s_1 > + < s_2 > + < s_1 s_2 s_3 >) + K_{32} < s_3 > & (3.2.6) \\ < s_1 s_2 s_3 > &= a_1 < s_2 s_3 > +a_2 < s_0 s_2 s_3 > & (3.2.7) \end{aligned}$$

With (3.1.5), (3.2.1), (3.2.4), (3.2.5), (3.2.6), (3.2.7) we have 6 equations and 6 unknowns (two of them are magnetizations, two of them are two spin correlations, two of them are three spin correlations.)

$$\begin{aligned} x_1 - 3K_{31}x_2 - K_{32}x_6 &= 0 \\ x_2 - a_2 x_1 &= x_1 \\ x_3 - (2K_{31} + K_{32})x_4 &= K_{31} \\ x_4 - a_1 x_2 - a_2 x_3 &= 0 \\ x_5 - (2K_{31} + K_{32})x_2 - K_{31}x_6 &= 0 \\ x_6 - a_1 x_4 - a_2 x_5 &= 0 \end{aligned} \tag{3.2.8}$$

where

$$\begin{aligned} x_1 &\equiv < s_0 > \\ x_2 &\equiv < s_1 >=< s_2 >=< s_3 > \\ x_3 &\equiv < s_0 s_1 >=< s_0 s_2 >=< s_0 s_3 > \\ x_4 &\equiv < s_1 s_2 >=< s_1 s_3 >=< s_2 s_3 > \\ x_5 &\equiv < s_0 s_1 s_2 >=< s_0 s_1 s_3 >=< s_0 s_2 s_3 > \\ x_6 &\equiv < s_1 s_2 s_3 > \end{aligned} \tag{3.2.9}$$

This system of equations can be represented by matrix equation $A.X = B$, where A is the coefficient matrix, X is the vector whose elements are unknowns and

B is the vector whose elements are the coefficients of the right hand side of the system

$$A = \begin{pmatrix} 1 & -3K_{31} & 0 & 0 & 0 & -K_{32} \\ -a_2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -(2K_{31}+K_{32}) & 0 & 0 \\ 0 & -a_1 & -a_2 & 1 & 0 & 0 \\ 0 & -(2K_{31}+K_{32}) & 0 & 0 & 1 & -K_{31} \\ 0 & 0 & 0 & -a_1 & -a_2 & 1 \end{pmatrix}$$

$$X = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{pmatrix} \qquad B = \begin{pmatrix} 0 \\ a_1 \\ K_{31} \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

One can solve this system easily with LU decomposition Method, Kramers Method or some other methods. We use Kramers Method to solve this system with Maple V R5 and we get the magnetizations and correlations as a function of temperature and external fields for various S-1/2 Ising systems by using (2.4.25), (2.4.26), (2.4.27) for the S-1/2 Ising systems with no external field, with external magnetic field and with transverse field.

For obtaining the temperature dependence of the effective field for the system with $z = 3$ we have to solve the self consistency equation (2.4.15). For this we have to obtain the central spin and the perimeter spin average magnetization namely x_1 and x_2 from the system of equations (3.2.8). When we apply the Kramer's Rule to the matrix A in this section we can get all the unknowns in terms of the coefficients. The coefficients are given by (2.4.24) and here we use the function (2.4.25) for the Ising system with $z = 3$ without external field.

After these, the temperature dependence of the effective field per spin is given by

$$y = \frac{1}{4}\ln(\frac{1}{2}e^{\frac{4}{x}} - e^{\frac{2}{x}} - \frac{1}{2} + \frac{1}{2}\sqrt{e^{\frac{8}{x}} - 4e^{\frac{6}{x}} + 2e^{\frac{4}{x}} + 4e^{\frac{2}{x}} - 3})x \qquad (3.2.10)$$

where $y = h/J$ and $x = kT/J$.

From (3.2.10) we can get the diagram of effective field per spin versus temperature. Since we have the effective field as a function of temperature from (3.2.10) then we can get the central spin magnetization as a function of temperature and we can draw the magnetization versus temperature curve. (Because we have solved all unknowns with matrix A). See Figure (3.1)

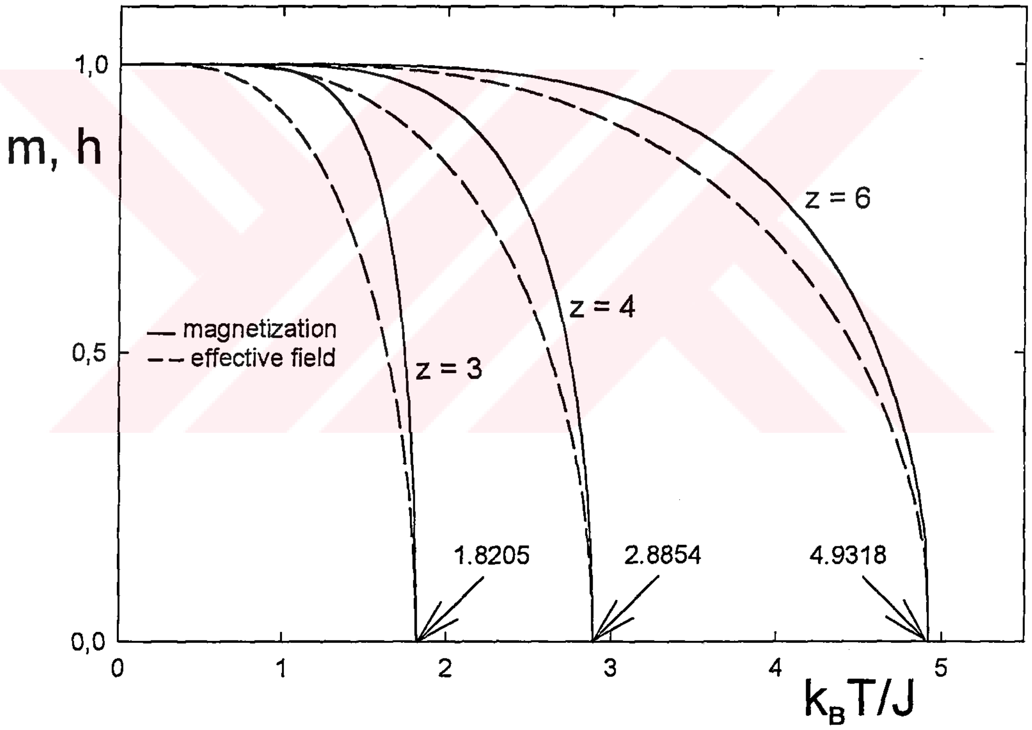

Figure 3.1: Magnetizations and effective fields versus temperature for different two dimensional lattices

As we can see from Figure (3.1) magnetization starts from 1 at low temperatures then shows sharp decreasing at certain temperature which is a characteristic property of the magnetic phase transition. Also we can see that the critical temperatures $T_c = 1.8205$ for honeycomb lattice, $T_c = 2.8854$ for square lattice and

$T_c = 4.9327$ for triangular lattice are same as the differential operator technique (and Bethe approximation) results. One interesting point is we do not have anti-Curie point in contrast to differential operator technique in the phase diagrams.

Again with the Kramer's rule we can get all correlations as a function of effective field and temperature, then their diagrams. See Figure (3.2) and Figure (3.3)

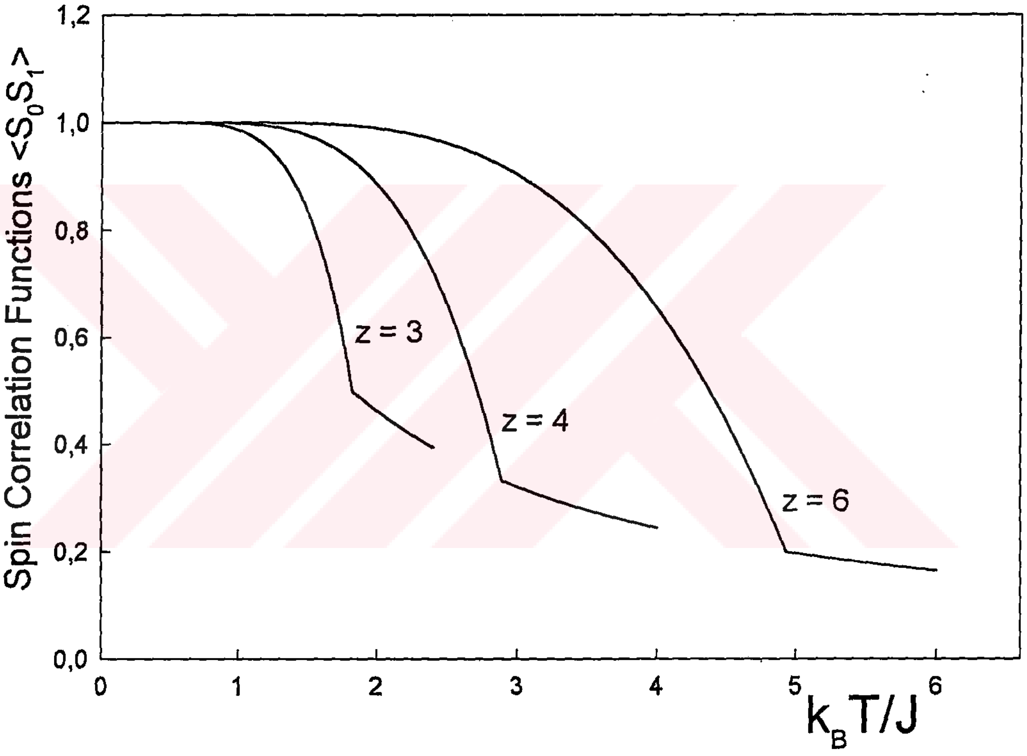

Figure 3.2: Two spin correlation functions versus temperature for different two dimensional lattices

We can see from Figure (3.2) that two spin correlation functions about the central spin are decreasing with temperature. After the critical temperatures this decreasing is slower than before the critical temperature. Since two spin correlation function is about the internal energy of the system, this behavior explains the behavior of the internal energy. At low temperatures two spin correlation functions show a maximum (i.e. the internal energy is minimum, thus the system has perfect order). While the temperature increases the correlations decreases for the three type of lattice. This means that the internal energy is increasing towards zero (i.e. the order of the system decreasing). After the critical temperature the increasing internal energy of the system is getting slower and while the temperature goes to infinity the internal energy of the system goes to zero. Also we can estimate from Figure (3.2) the behavior of the specific heat since the specific heat is the derivative of the internal energy with respect to temperature and the internal energy is the negative of the two spin correlation functions. From this we can estimate the divergence-like behavior of the specific heat at the critical temperature.

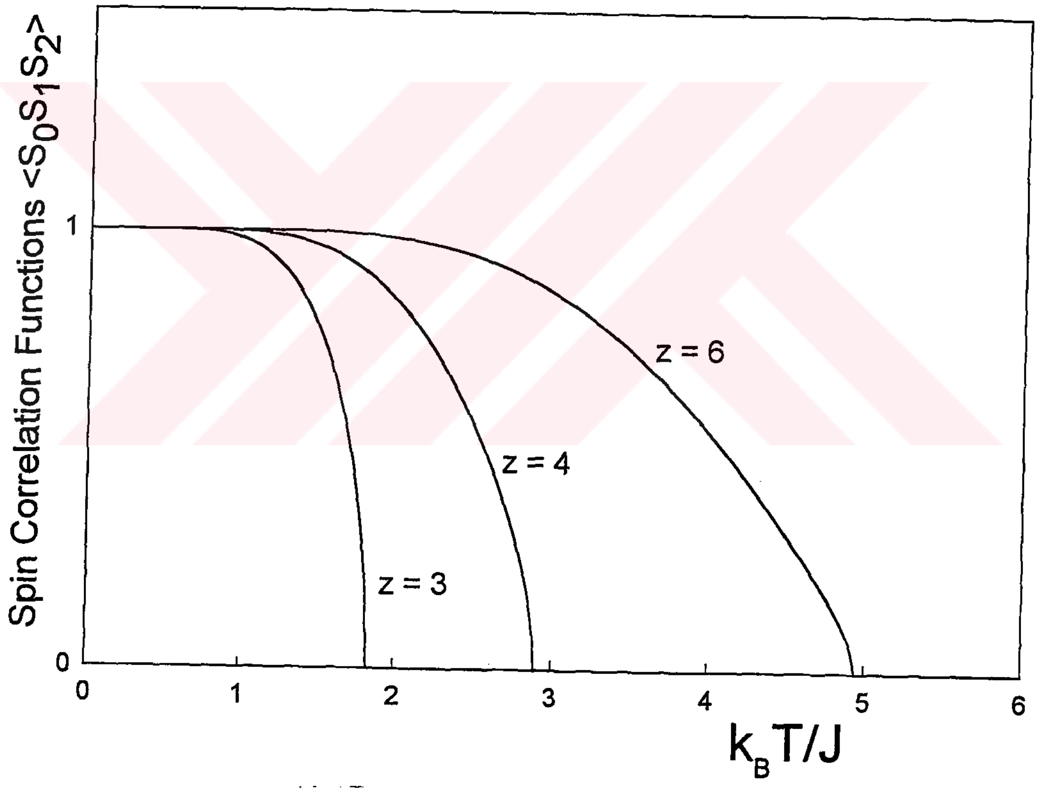

Figure 3.3: Three spin correlation functions versus temperature for different two dimensional lattices

From Figure (3.3) firstly we see the different behavior of the three spin correlation functions about the central spin from the two spin correlation function; they go to the zero while the temperature goes to the critical temperature.

From the formulation we can say that the higher correlations (e.g. four, five spin correlation functions) are decreasing faster than the two and three spin correlation functions respectively.

From (3.5.2) and (3.5.3)we can obtain the internal energy and specific heat as a function of temperature. Finally we can get the temperature dependence of the susceptibility from (3.5.1)

3.3 Square lattice

The calculations are same as the honeycomb lattice. We start by expanding (3.1.3) for $z = 4$ and take the odd operators only

$$\begin{aligned} < s_0 > &= K_{41}(< s_1 > + < s_2 > + < s_3 > + < s_4 >) + \\ & K_{42}(< s_1 s_2 s_3 > + < s_1 s_2 s_4 > \\ & + < s_1 s_3 s_4 > + < s_2 s_3 s_4 >) \end{aligned} \tag{3.3.1}$$

The coefficients K_{41} and K_{42} are given by (2.4.24) and the perimeter spin magnetization, from (3.1.5)

$$< s_1 >= a_1 + a_2 < s_0 > \tag{3.3.2}$$

a_1, a_2 are given by (2.4.8). for $z = 4$ equal correlations are as follows

$$\begin{aligned} < s_0 s_1 > &= < s_0 s_2 >=< s_0 s_3 >=< s_0 s_4 > \\ < s_1 s_2 > &= < s_1 s_3 >=< s_1 s_4 >=< s_2 s_3 > \\ &= < s_2 s_4 >=< s_3 s_4 > \\ < s_0 s_1 s_2 > &= < s_0 s_1 s_3 >=< s_0 s_1 s_4 >=< s_0 s_2 s_3 > \\ &= < s_0 s_2 s_4 >=< s_0 s_3 s_4 > \\ < s_1 s_2 s_3 > &= < s_1 s_2 s_4 >=< s_1 s_3 s_4 >=< s_2 s_3 s_4 > \\ < s_0 s_1 s_2 s_3 > &= < s_0 s_1 s_2 s_4 >=< s_0 s_1 s_3 s_4 >=< s_0 s_2 s_3 s_4 > \end{aligned} \tag{3.3.3}$$

Also from (2.4.5)

$$< s_1 >=< s_2 >=< s_3 >=< s_4 > \tag{3.3.4}$$

From (3.3.1) and (3.3.2), with the condition $s^2 = 1$ we can generate the equations of correlations as follows

$$\begin{aligned}
< s_0 s_1 > &= K_{41}(1+ < s_1 s_2 > \\
&\quad + < s_1 s_3 > + < s_1 s_4 >)+ \\
&\quad K_{42}(< s_2 s_3 > + < s_2 s_4 > \\
&\quad + < s_3 s_4 > + < s_1 s_2 s_3 s_4 >) \\
< s_1 s_2 > &= a_1 < s_2 > +a_2 < s_0 s_2 > \\
< s_0 s_1 s_2 > &= K_{41}(< s_1 > + < s_2 > \\
&\quad + < s_1 s_2 s_3 > + < s_1 s_2 s_4 >) \\
&\quad +K_{42}(< s_3 > + < s_4 > \\
&\quad + < s_2 s_3 s_4 > + < s_1 s_3 s_4 >) \\
< s_1 s_2 s_3 > &= a_1 < s_2 s_3 > +a_2 < s_0 s_2 s_3 > \\
< s_0 s_1 s_2 s_3 > &= K_{41}(< s_1 s_3 > + < s_2 s_3 > \\
&\quad + < s_1 s_2 > + < s_1 s_2 s_3 s_4 >) \\
&\quad +K_{42}(1+ < s_3 s_4 > + < s_2 s_4 > + < s_1 s_4 >) \\
< s_1 s_2 s_3 s_4 > &= a_1 < s_2 s_3 s_4 > +a_2 < s_0 s_2 s_3 s_4 >
\end{aligned} \tag{3.3.5}$$

With (3.3.1), (3.3.2) and (3.3.5) we have 8 equations and 8 unknowns as follows

$$\begin{aligned}
x_1 - 4K_{41}x_2 - 4K_{42}x_6 &= 0 \\
x_2 - a_2 x_1 &= a_1 \\
x_3 - 3(K_{41} + K_{42})x_4 - K_{42}x_8 &= K_{41} \\
x_4 - a_1 x_2 - a_2 x_3 &= 0 \\
x_5 - 2(K_{41} + K_{42}) - 2(K_{41} + K_{42})x_6 &= 0 \\
x_6 - a_1 x_4 - a_2 x_5 &= 0 \\
x_7 - 3(K_{41} + K_{42})x_4 - K_{41}x_8 &= K_{42} \\
x_8 - a_1 x_6 - a_2 x_7 &= 0
\end{aligned} \tag{3.3.6}$$

where

$$\begin{aligned}
x_1 &\equiv\ < s_0 > \\
x_2 &\equiv\ < s_1 >=< s_2 >=< s_3 >=< s_4 > \\
x_3 &\equiv\ < s_0 s_1 >=< s_0 s_2 >=< s_0 s_3 >=< s_0 s_4 > \\
x_4 &\equiv\ < s_1 s_2 >=< s_1 s_3 >=< s_1 s_4 >=< s_2 s_3 > \\
&=\ < s_2 s_4 >=< s_3 s_4 > \\
x_5 &\equiv\ < s_0 s_1 s_2 >=< s_0 s_1 s_3 >=< s_0 s_1 s_4 >=< s_0 s_2 s_3 > \\
&=\ < s_0 s_2 s_4 >=< s_0 s_3 s_4 > \\
x_6 &\equiv\ < s_1 s_2 s_3 >=< s_1 s_2 s_4 >=< s_1 s_3 s_4 >=< s_2 s_3 s_4 > \\
x_7 &\equiv\ < s_0 s_1 s_2 s_3 >=< s_0 s_1 s_2 s_4 >=< s_0 s_1 s_3 s_4 >=< s_0 s_2 s_3 s_4 > \\
x_8 &\equiv\ < s_1 s_2 s_3 s_4 >
\end{aligned} \tag{3.3.7}$$

Again we use the Kramer's Method to solve this system with Maple V R5 and we get the magnetizations and correlations as a function of temperature and external fields for various S-1/2 Ising systems by using (2.4.25), (2.4.26), (2.4.27) for the S-1/2 Ising systems with no external field, with external magnetic field and with transverse field.

By getting x_1 and x_2 (which are the central spin average magnetization and the perimeter spin average magnetization) from (3.3.6) system of equations and substituting them in (2.4.15) we can get the effective field as a function of temperature

$$y = \frac{1}{6}\ln\left(\frac{1}{2}e^{\frac{6}{x}} - \frac{3}{2}e^{\frac{2}{x}} + \frac{1}{2}\sqrt{e^{\frac{6}{x}} - 6e^{\frac{8}{x}} + 9e^{\frac{4}{x}} - 4}\right)x \tag{3.3.8}$$

where $y = h/J$ and $x = kT/J$. Since all magnetization, correlations and thermodynamic functions depend on the effective field and temperature we can get these quantities as a function of temperature via (3.3.8)

The diagrams of the effective field, magnetization, correlations and thermodynamic functions versus temperature can be obtained with the same procedures as honeycomb lattice. See Figure (3.1), Figure (3.2) and Figure (3.3).

3.4 Triangular lattice

Again we start by expanding (3.1.3) for $z = 6$ and take the odd operators only

$$\begin{aligned}
< s_0 > &= K_{61}(< s_1 > + < s_2 > + < s_3 > \\
&+ < s_4 > + < s_5 > + < s_6 >) \\
&+K_{62}(< s_1 s_2 s_3 > + < s_1 s_2 s_4 > + < s_1 s_2 s_5 > \\
&+ < s_1 s_2 s_6 > + < s_1 s_3 s_4 > + < s_1 s_3 s_5 > \\
&+ < s_1 s_3 s_6 > + < s_1 s_4 s_5 > + < s_1 s_4 s_6 > \\
&+ < s_1 s_5 s_6 > + < s_2 s_3 s_4 > + < s_2 s_3 s_5 > \\
&+ < s_2 s_3 s_6 > + < s_2 s_4 s_5 > + < s_2 s_4 s_6 > \\
&+ < s_2 s_5 s_6 > + < s_3 s_4 s_5 > + < s_3 s_4 s_6 > \\
&+ < s_3 s_5 s_6 > + < s_4 s_5 s_6 >) \\
&+K_{63}(< s_1 s_2 s_3 s_4 s_5 > + < s_1 s_2 s_3 s_4 s_6 > \\
&+ < s_1 s_2 s_3 s_5 s_6 > + < s_1 s_2 s_4 s_5 s_6 > \\
&+ < s_1 s_3 s_4 s_5 s_6 > + < s_2 s_3 s_4 s_5 s_6 >) \\
< s_1 > &= a_1 + a_2 < s_0 > \\
< s_0 s_1 > &= K_{61}(1 + < s_1 s_2 > + < s_1 s_3 > + < s_1 s_4 > \\
&+ < s_1 s_5 > + < s_1 s_6 >) \\
&+K_{62}(< s_2 s_3 > + < s_2 s_4 > + < s_2 s_5 > \\
&+ < s_2 s_6 > + < s_3 s_4 > + < s_3 s_5 > \\
&+ < s_3 s_6 > + < s_4 s_5 > + < s_4 s_6 > \\
&+ < s_5 s_6 > + < s_1 s_2 s_3 s_4 > + < s_1 s_2 s_3 s_5 > \\
&+ < s_1 s_2 s_3 s_6 > + < s_1 s_2 s_4 s_5 > + < s_1 s_2 s_4 s_6 > \\
&+ < s_1 s_2 s_5 s_6 > + < s_1 s_3 s_4 s_5 > + < s_1 s_3 s_4 s_6 > + \\
&< s_1 s_3 s_5 s_6 > + < s_1 s_4 s_5 s_6 >) + \\
&K_{63}(< s_2 s_3 s_4 s_5 > + < s_2 s_3 s_4 s_6 > + < s_2 s_3 s_5 s_6 > \\
&+ < s_2 s_4 s_5 s_6 > + < s_3 s_4 s_5 s_6 > + < s_1 s_2 s_3 s_4 s_5 s_6 >) \\
< s_1 s_2 > &= a_1 < s_2 > + a_2 < s_0 s_2 >
\end{aligned} \tag{3.4.1}$$

$$
\begin{aligned}
< s_0 s_1 s_2 > \quad &= \quad K_{61}(< s_2 > + < s_1 > + < s_1 s_2 s_3 > \\
&+ < s_1 s_2 s_4 > + < s_1 s_2 s_5 > + < s_1 s_2 s_6 >) \\
&+ K_{62}(< s_3 > + < s_4 > + < s_5 > + < s_6 > \\
&+ < s_2 s_3 s_4 > + < s_2 s_3 s_5 > + < s_2 s_3 s_6 > \\
&+ < s_2 s_4 s_5 > + < s_2 s_4 s_6 > + < s_2 s_5 s_6 > \\
&+ < s_1 s_3 s_4 > + < s_1 s_3 s_5 > + < s_1 s_3 s_6 > \\
&+ < s_1 s_4 s_5 > + < s_1 s_4 s_6 > + < s_1 s_5 s_6 > \\
&+ < s_1 s_2 s_3 s_4 s_5 > + < s_1 s_2 s_3 s_4 s_6 > \\
&+ < s_1 s_2 s_3 s_5 s_6 > + < s_1 s_2 s_4 s_5 s_6 >) \\
&+ K_{63}(< s_3 s_4 s_5 > + < s_3 s_4 s_6 > + < s_3 s_5 s_6 > \\
&+ < s_4 s_5 s_6 > + < s_2 s_3 s_4 s_5 s_6 > + < s_1 s_3 s_4 s_5 s_6 >) \\
< s_1 s_2 s_3 > \quad &= \quad a_1 < s_2 s_3 > + a_2 < s_0 s_2 s_3 > \\
< s_0 s_1 s_2 s_3 > \quad &= \quad K_{61}(< s_2 s_3 > + < s_1 s_3 > + < s_1 s_2 > \\
&+ < s_1 s_2 s_3 s_4 > + < s_1 s_2 s_3 s_5 > + < s_1 s_2 s_3 s_6 >) \\
&+ K_{62}(1 + < s_3 s_4 > + < s_3 s_5 > \\
&+ < s_3 s_6 > + < s_2 s_4 > + < s_2 s_5 > \\
&+ < s_2 s_6 > + < s_2 s_3 s_4 s_5 > + < s_2 s_3 s_4 s_6 > \\
&+ < s_2 s_3 s_5 s_6 > + < s_1 s_4 > + < s_1 s_5 > \\
&+ < s_1 s_6 > + < s_1 s_3 s_4 s_5 > + < s_1 s_3 s_4 s_6 > \\
&+ < s_1 s_3 s_5 s_6 > + < s_1 s_2 s_4 s_5 > + < s_1 s_2 s_4 s_6 > \\
&+ < s_1 s_2 s_5 s_6 > + < s_1 s_2 s_3 s_4 s_5 s_6 >) \\
&+ K_{63}(< s_4 s_5 > + < s_4 s_6 > + < s_5 s_6 > \\
&+ < s_3 s_4 s_5 s_6 > + < s_2 s_4 s_5 s_6 > + < s_1 s_4 s_5 s_6 >) \\
< s_1 s_2 s_3 s_4 > \quad &= \quad a_1 < s_2 s_3 s_4 > + a_2 < s_0 s_2 s_3 s_4 >
\end{aligned}
$$

$$
\begin{aligned}
< s_0 s_1 s_2 s_3 s_4 > \quad &= \quad K_{61}(< s_2 s_3 s_4 > + < s_1 s_3 s_4 > + < s_1 s_2 s_4 > \\
&+ < s_1 s_2 s_3 > + < s_1 s_2 s_3 s_4 s_5 > + < s_1 s_2 s_3 s_4 s_6 >) \\
&+K_{62}(< s_4 > + < s_3 > + < s_3 s_4 s_5 > \\
&+ < s_3 s_4 s_6 > + < s_2 > + < s_2 s_4 s_5 > \\
&+ < s_2 s_4 s_6 > + < s_2 s_3 s_5 > + < s_2 s_3 s_6 > \\
&+ < s_2 s_3 s_4 s_5 s_6 > + < s_1 > + < s_1 s_4 s_5 > \\
&+ < s_1 s_4 s_6 > + < s_1 s_3 s_5 > + < s_1 s_3 s_6 > \\
&+ < s_1 s_3 s_4 s_5 s_6 > + < s_1 s_2 s_5 > + < s_1 s_2 s_6 > \\
&+ < s_1 s_2 s_4 s_5 s_6 > + < s_1 s_2 s_3 s_5 s_6 >)+ \\
&+K_{63}(< s_5 > + < s_6 > + < s_4 s_5 s_6 > \\
&+ < s_3 s_5 s_6 > + < s_2 s_5 s_6 > + < s_1 s_5 s_6 >) \\
< s_1 s_2 s_3 s_4 s_5 > \quad &= \quad a_1 < s_2 s_3 s_4 s_5 > +a_2 < s_0 s_2 s_3 s_4 s_5 > \\
< s_0 s_1 s_2 s_3 s_4 s_5 > \quad &= \quad K_{61}(< s_2 s_3 s_4 s_5 > + < s_1 s_3 s_4 s_5 > + < s_1 s_2 s_4 s_5 > \\
&+ < s_1 s_2 s_3 s_5 > + < s_1 s_2 s_3 s_4 > + < s_1 s_2 s_3 s_4 s_5 s_6 >)+ \\
&K_{62}(< s_4 s_5 > + < s_3 s_5 > + < s_3 s_4 > \\
&+ < s_3 s_4 s_5 s_6 > + < s_2 s_5 > + < s_2 s_4 > \\
&+ < s_2 s_4 s_5 s_6 > + < s_2 s_3 > + < s_2 s_3 s_5 s_6 > \\
&+ < s_2 s_3 s_4 s_6 > + < s_1 s_5 > + < s_1 s_4 > \\
&+ < s_1 s_4 s_5 s_6 > + < s_1 s_3 > + < s_1 s_3 s_5 s_6 > \\
&+ < s_1 s_3 s_4 s_6 > + < s_1 s_2 > + < s_1 s_2 s_5 s_6 > \\
&+ < s_1 s_2 s_4 s_6 > + < s_1 s_2 s_3 s_6 >) \\
&+K_{63}(1+ < s_5 s_6 > + < s_4 s_6 > \\
&+ < s_3 s_6 > + < s_2 s_6 > + < s_1 s_6 >) \\
< s_1 s_2 s_3 s_4 s_5 s_6 > \quad &= \quad a_1 < s_2 s_3 s_4 s_5 s_6 > +a_2 < s_0 s_2 s_3 s_4 s_5 s_6 >
\end{aligned}
$$

With (3.4.1) 12 equations are as follows

$$
\begin{aligned}
& x_1 - 6K_{61}x_2 - 20K_{62}x_6 - \\
& 6K_{63}x_{10} && = 0 \\
& x_2 - a_2x_1 && = a_1 \\
& x_3 - (5K_{61} + 10K_{62})x_4 - (10K_{62} + \\
& 5K_{63})x_8 - K_{63}x_{12} && = K_{61} \\
& x_4 - a_1x_2 - a_2x_3 && = 0 \\
& x_5 - (2K_{61} + 4K_{62})x_2 - (4K_{61} + \\
& 12K_{62} + 4K_{63})x_6 - (4K_{61} + 2K_{63})x_{10} && = 0 \\
& x_6 - a_1x_4 - a_2x_5 && = 0 \\
& x_7 - (3K_{61} + 9K_{62} + 3K_{63})x_4 - \\
& (3K_{61} + 9K_{62} + 3K_{63})x_8 - K_{61}x_{12} && = K_{62} \\
& x_8 - a_1x_6 - a_2x_7 && = 0 \\
& x_9 - 4K_{62}x_2 - (4K_{61} + 12K_{62})x_6 - \\
& (2K_{61} + 4K_{62})x_{10} && = 0 \\
& x_{10} - a_1x_8 - a_2x_9 && = 0 \\
& x_{11} - (10K_{62} + 5K_{63})x_4 - (5K_{61} + \\
& 10K_{62})x_8 - K_{61}x_{12} && = K_{63} \\
& x_{12} - a_1x_{10} - a_2x_{11} && = 0
\end{aligned}
\tag{3.4.2}
$$

where

$$\begin{aligned}
x_1 &\equiv\ < s_0 > \\
x_2 &\equiv\ < s_1 >=< s_2 >=< s_3 >=< s_4 >=< s_5 >=< s_6 > \\
x_3 &\equiv\ < s_0s_1 >=< s_0s_2 >=< s_0s_3 > \\
&=\ < s_0s_4 >=< s_0s_5 >=< s_0s_6 > \\
x_4 &\equiv\ < s_1s_2 >=< s_1s_3 >=< s_1s_4 >=< s_1s_5 > \\
&=\ < s_1s_6 >=< s_2s_3 >=< s_2s_4 >=< s_2s_5 > \\
&=\ < s_2s_6 >=< s_3s_4 >=< s_3s_5 >=< s_3s_6 > \\
&=\ < s_4s_5 >=< s_4s_6 >=< s_5s_6 > \\
x_5 &\equiv\ < s_0s_1s_2 >=< s_0s_1s_3 >=< s_0s_1s_4 > \\
&=\ < s_0s_1s_5 >=< s_0s_1s_6 >=< s_0s_2s_3 > \\
&=\ < s_0s_2s_4 >=< s_0s_2s_5 >=< s_0s_2s_6 > \\
&=\ < s_0s_3s_4 >=< s_0s_3s_5 >=< s_0s_3s_6 > \\
&=\ < s_0s_4s_5 >=< s_0s_4s_6 >=< s_0s_5s_6 > \\
x_6 &\equiv\ < s_1s_2s_3 >=< s_1s_2s_4 >=< s_1s_2s_5 > \\
&=\ < s_1s_2s_6 >=< s_1s_3s_4 >=< s_1s_3s_5 > \\
&=\ < s_1s_3s_6 >=< s_1s_4s_5 >=< s_1s_4s_6 > \\
&=\ < s_1s_5s_6 >=< s_2s_3s_4 >=< s_2s_3s_5 > \\
&=\ < s_2s_3s_6 >=< s_2s_4s_5 >=< s_2s_4s_6 > \\
&=\ < s_2s_5s_6 >=< s_3s_4s_5 >=< s_3s_4s_6 > \\
&=\ < s_3s_5s_6 >=< s_4s_5s_6 > \\
x_7 &\equiv\ < s_0s_1s_2s_3 >=< s_0s_1s_2s_4 >=< s_0s_1s_2s_5 > \\
&=\ < s_0s_1s_2s_6 >=< s_0s_1s_3s_4 >=< s_0s_13s_5 > \\
&=\ < s_0s_1s_3s_6 >=< s_0s_1s_4s_5 >=< s_0s_1s_4s_6 > \\
&=\ < s_0s_1s_5s_6 >=< s_0s_2s_3s_4 >=< s_0s_2s_3s_5 > \\
&=\ < s_0s_2s_3s_6 >=< s_0s_2s_4s_5 >=< s_0s_2s_4s_6 > \\
&=\ < s_0s_2s_5s_6 >=< s_0s_3s_4s_5 >=< s_0s_3s_4s_6 > \\
&=\ < s_0s_3s_5s_6 >=< s_0s_4s_5s_6 > \\
x_8 &\equiv\ < s_1s_2s_3s_4 >=< s_1s_2s_3s_5 >=< s_1s_2s_3s_6 >=< s_1s_2s_4s_5 > \\
&=\ < s_1s_2s_4s_6 >=< s_1s_2s_5s_6 >=< s_1s_3s_4s_5 >=< s_1s_3s_4s_6 > \\
&=\ < s_1s_3s_5s_6 >=< s_1s_4s_5s_6 >=< s_2s_3s_4s_5 >=< s_2s_3s_4s_6 > \\
&=\ < s_2s_3s_5s_6 >=< s_2s_4s_5s_6 >
\end{aligned} \tag{3.4.3}$$

$$\begin{aligned}
x_9 &\equiv < s_0s_1s_2s_3s_4 >=< s_0s_1s_2s_3s_5 >=< s_0s_1s_2s_3s_6 > \\
&= < s_0s_1s_2s_4s_5 >=< s_0s_1s_2s_4s_6 >=< s_0s_1s_2s_5s_6 > \\
&= < s_0s_1s_3s_4s_5 >=< s_0s_1s_3s_4s_6 >=< s_0s_1s_3s_5s_6 > \\
&= < s_0s_1s_4s_5s_6 >=< s_0s_2s_3s_4s_5 >=< s_0s_2s_3s_4s_6 > \\
&= < s_0s_2s_3s_5s_6 >=< s_0s_2s_4s_5s_6 > \\
x_{10} &\equiv < s_1s_2s_3s_4s_5 >=< s_1s_2s_3s_4s_6 >=< s_1s_2s_3s_5s_6 > \\
&= < s_1s_2s_4s_5s_6 >=< s_1s_3s_4s_5s_6 >=< s_2s_3s_4s_5s_6 > \\
x_{11} &\equiv < s_0s_1s_2s_3s_4s_5 >=< s_0s_1s_2s_3s_4s_6 >=< s_0s_1s_2s_3s_5s_6 > \\
&= < s_0s_1s_2s_4s_5s_6 >=< s_0s_1s_3s_4s_5s_6 >=< s_0s_2s_3s_4s_5s_6 > \\
x_{12} &\equiv < s_1s_2s_3s_4s_5s_6 >
\end{aligned}$$

Similar to the honeycomb and square lattice systems, these equations can be represented by matrices an solved for various systems.

With a similar procedure explained above (for honeycomb and square lattices) we can get the magnetization, correlations and thermodynamic functions as a function of temperature; with self-consistency condition (2.4.15) and substituting x_1, x_2 which are obtained by solving system of equations (3.4.2). Then we find the effective field for triangular lattice

$$\begin{aligned}
y &= \frac{1}{10}\ln\left(\frac{1}{4}e^{\frac{10}{x}} - \frac{5}{4}e^{\frac{2}{x}} + \frac{1}{4}M\right. \\
&+ \left.\frac{1}{4}\sqrt{2e^{\frac{20}{x}} - 20e^{\frac{12}{x}} + 2e^{\frac{10}{x}}M + 10e^{\frac{4}{x}} - 10e^{\frac{2}{x}}M + 20e^{\frac{8}{x}} - 12}\right) x \qquad (3.4.4)
\end{aligned}$$

where

$$M = \sqrt{e^{\frac{20}{x}} - 10e^{\frac{12}{x}} - 15e^{\frac{4}{x}} + 20e^{\frac{8}{x}} + 4}$$

See Figure (3.1), Figure (3.2) and Figure (3.3).

3.5 Thermodynamic properties

Once the magnetization is obtained from the formulation as a function of the effective field, temperature and the external fields acting on the system and effective field as a function of the temperature and the external fields then we can obtain the magnetization as a function of the temperature and the external fields. Thus we can obtain the susceptibility as a function of temperature and external fields with

$$\chi(T) = \frac{\partial m(T,H)}{\partial H} \tag{3.5.1}$$

The internal energy per spin of the system is from (2.5.2),

$$U/N = -J(< s_0 s_1 > + < s_0 s_2 > + ... + < s_0 s_z >) - H(< s_0 >) \tag{3.5.2}$$

Indeed (3.5.2) is same as (2.5.3). But this time instead of using (2.5.4) we use the correlations which are obtained by the Kramer's Rule from the matrix A. Thus we can obtain the internal energy per spin easily then we can obtain the specific heat via

$$C(T) = \frac{\partial U}{\partial T} \tag{3.5.3}$$

Then we can obtain the complete description (i.e. the dependence of magnetization, correlations and thermodynamic functions as a function to the temperature and eternal fields) of our system easily in this formulation.

3.6 Spin-1/2 Ising systems under the transverse field

In the S-1/2 Ising systems with transverse field the Hamiltonian is

$$H = -J \sum_{<i,j>} s_i^z s_j^z - \Omega \sum_i s_i^x \tag{3.6.1}$$

where Ω is the transverse field acting on the system and s_i^x is the spin operator's x component at a site i. We have to solve the system of equations (3.2.8), (3.3.6), (3.4.2) with parameters (2.4.24) and function (2.4.27) for obtaining the magnetization and correlations as a function of effective field, transverse field and temperature of the honeycomb, square and triangular lattices respectively. Then by solving the self-consistency equation (2.4.15) for fixed transverse field we can get the temperature dependence of the effective field. Thus we can determine the temperature dependence of the magnetization and the correlations for certain transverse field.

For determining the transverse field dependence of the critical temperature we must solve the self-consistency equation (2.4.15) with the assumption that the effective field is very small near the critical temperature. Then substituting zero (or a small value) effective field in (2.4.15) we can get the equation with two unknowns : one is the critical temperature, and the other is the transverse field. Then by solving this equation for fixed transverse fields we can get the critical temperatures in that transverse field. In this way we can plot the critical temperature vs transverse field curves for various two dimensional lattices. See Figure (3.4)

From Figure (3.4) we can see the behavior of the critical temperature while the transverse field increases. It slowly decreases for small transverse fields then at a certain transverse fields value the critical temperatures of the three different systems have sharp decreasing. Finally at critical transverse field values three systems critical temperatures takes the value zero. Due to this interesting behavior of the critical temperature, transverse Ising systems are important.

While the critical temperatures at a zero transverse field are same as the differential operator technique's, the critical values of the transverse fields are a little higher than the differential operator technique's. The values of the critical transverse fields are $\frac{\Omega_c}{J} = 1.3785$ for honeycomb lattice, $\frac{\Omega_c}{J} = 2.4434$ for square lattice and $\frac{\Omega_c}{J} = 4.5005$ for triangular lattice. These values can be compared with the values which are obtained by some other methods : Mean field approximation ($\frac{\Omega_c}{J} = 3$ for honeycomb lattice, $\frac{\Omega_c}{J} = 4$ for square lattice and $\frac{\Omega_c}{J} = 6$ for triangular lattice), pair approximation (Ma & Ma, 1993)) ($\frac{\Omega_c}{J} = 2$ for honeycomb

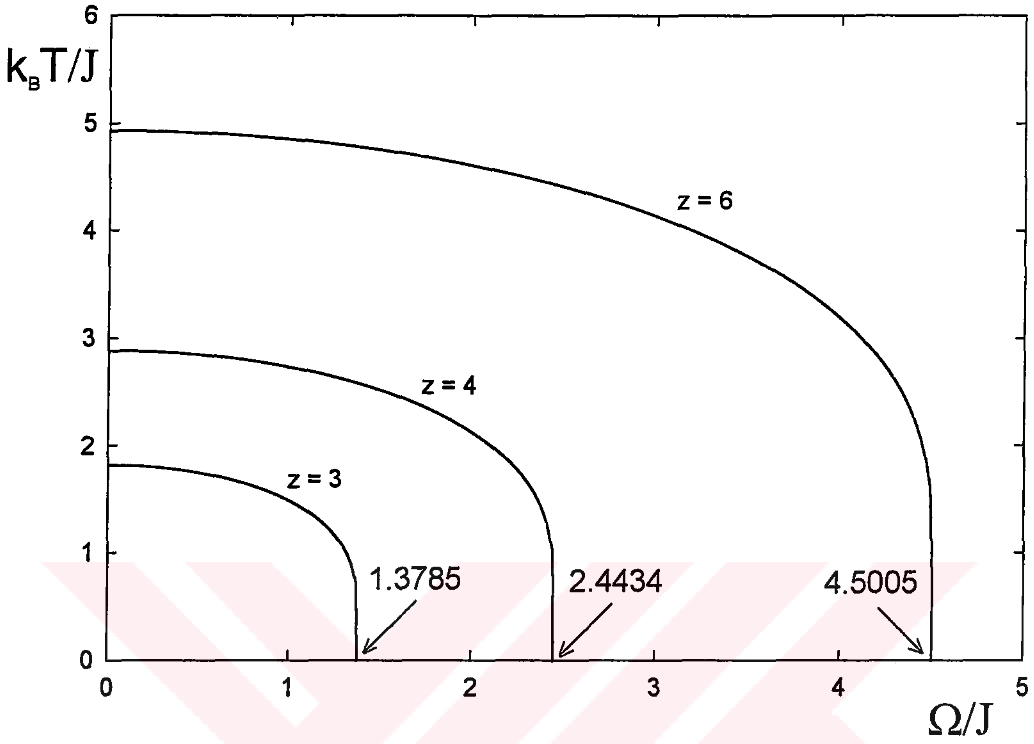

Figure 3.4: The phase diagram of the spin-1/2 transverse Ising model plotted in the $(\frac{kT}{J}, \frac{\Omega}{J})$ space.

lattice, $\frac{\Omega_c}{J} = 3$ for square lattice and $\frac{\Omega_c}{J} = 5$ for triangular lattice), effective field theory (Tamura et al., 1984,Elkouraychi et al, 1995) ($\frac{\Omega_c}{J} = 1.8300$ for honeycomb lattice, $\frac{\Omega_c}{J} = 2.7520$ for square lattice and $\frac{\Omega_c}{J} = 4.7060$ for triangular lattice), differential operator technique (Kaneyoshi, 1999) ($\frac{\Omega_c}{J} = 1.2268$ for honeycomb lattice, $\frac{\Omega_c}{J} = 2.3934$ for square lattice and $\frac{\Omega_c}{J} = 4.4813$ for triangular lattice) and the renormalization group technique (Santos, 1982) ($\frac{\Omega_c}{J} = 1.5552$ for square lattice)

CHAPTER FOUR

CONCLUSIONS

In this work, we have studied the effective field theory (EFT) with correlations on honeycomb, square and triangular lattices in which attention is focused on a cluster comprising a central spin, labeled 0, and the z nearest-neighbor spins with which it directly interacts. With the use of differential operator technique and Ising spin identity, we have derived individually a set of linear equations for the spin-1/2 Ising systems with three coordination numbers z ($z = 3, 4, 6$). In the spin-1/2 Ising model, solution of the set of linear equations derived individually for the Ising systems gives the thermal variations of the spin correlation functions, the parameter h and the magnetization m.

After defining the fundamental concepts of the phase transition (critical phenomena) and summarizing the fundamental properties of the Ising model in chapter one, in chapter two we give briefly the differential operator technique (its sources, applications to different Ising systems, etc.). In chapter three we have developed a simple new technique under the differential operator technique where instead of using decoupling approximation ($< s_1 s_2 s_3 ... s_z > = < s_1 >< s_2 >< s_3 > ... < s_z >$) by calculating these correlations in differential operator technique. In this way we get the system of equations about three, two dimensional Ising systems which have $3, 4, 6$ number of nearest neighbor spins. Finally we get the phase diagrams of the two dimensional systems under no magnetic field and under the transverse field, in chapter three.

This new technique allows us to determine all correlations in our system, thus we get easily the internal energy which consist of the average of two spin correlation functions for those systems under no magnetic field.

Although we do not use the decoupling approximation in our technique we find critical temperatures which are the same as the Bethe approximation (and Kaneyoshi's differential operator technique also). But we can calculate the correlations easily within our technique and then the internal energy. Thus, for instance if we use Hamiltonian (1.2.1) by taking the first three terms which is investigated by another method in Doczi-Reger & Hemmer, 1981 we can easily get the two and three spin correlation functions then internal energy and specific heat. Or we can investigate the Ising system with two spin interactions and four spin interactions on the square lattice which is investigated in (Horiguchi, 1985) by another method we can easily obtain the two and four spin correlations and then internal energy and specific heat.

Besides our results about the critical temperatures (which are the same as the Bethe approximation's results) with our method only the critical values of $\frac{\Omega}{J}$ are a little higher than that of Kaneyoshi's critical values (Kaneyoshi, 1999) in the transverse field spin-1/2 Ising model.

On the other hand the anti-Curie point behaviour has not been observed in our systems whereas those were usually observed in the Bethe-Peierls approximation at low temperature.

The reasons of our critical values being as same as the Bethe approximation results (which is the best approximation for Ising systems as far as we know) are due to the effective field. Although we do not take the decoupling approximation in our method we still work with an effective field concept. We choose a central spin and calculate exactly the interactions of this central spin with its z neighbors, but we do not calculate the neighbor spin's interactions with spins which are outside the cluster exactly.

This method can be applied to a large variety of Ising systems. But this time we encounter some difficulties. The number of equations are increasing in spin-1 and higher spin systems. Besides this with higher spins we have to use approximated Van der Waerden identity instead of (2.2.8). With increasing number of equations we must solve the system of equations numerically. In this thesis we have solved our system of equations for spin-1/2 systems analytically. In a certain spin-s system the external fields do not effect the number of equations but effect the function $f(x)$. This time we may need some numerical calculations instead of analytical calculations also.

REFERENCES

Bak, P. & Boehm, J. von (1980). Ising model with solitons, phasons, and "the devil's staircase". Phys. Rev. B, 21, 5297-5308.

Baxter, R. J. & Enting, I. G. (1964) .399th solution of the Ising model. J. Phys. A, 11, 2463-2473.

Bethe, H. A. (1935). Proc. Roy. Soc. London A, 150, 552.

Blume, H. et al. (1971). Ising model for the λ transition and phase seperation in $^3He -^4 He$ mixtures. Phys. Rev. A, 4, 1071-1077.

Bragg, W. L. & Williams, E. J. (1934). Proc. Roy. Soc. London A, 145, 699.

Bragg, W. L. & Williams, E. J. (1935). Proc. Roy. Soc. London A, 151, 540.

Callen, H. B. (1963). A note on Green functions and the Ising model. Phys. Lett., 4, 161.

Doczi-Reger, J. & Hemmer, P. C. (1981). Second order phase transition in triangular Ising models with two and three spin interactions. Physica A, 109, 541-554.

Dresden, M. (1988). Kramers contributions to statistical-mechanics. Physics Today, September,1988, 26-33.

Elkouraychi, A. et al.(1995). On the theory of the transverse Ising-model with arbitrary spin. Physica A, 213, 576-586.

Gofman, M. et al. (1996). Critical behavior of the random field Ising model. Phys. Rev. B, 53, 6362-6384.

Goldenfeld, N. (1992). Lectures on Phase Transitions and the Renormalization Group. Addison-Wesley Publishing Company.

Honmura, R. & Kaneyoshi, T. (1979). Contribution to the new type of effective-field theory of the Ising-model. J. Phys. C, 12, 3979-3992.

Horiguchi, T. (1985). Ising model with two spin interactions and four spin interactions on the square lattice. Physica A, 130, 194-204.

Hurst, C. A. & Green, H. S. (1960). New solution of the Ising problem for a rectangular lattice. J. Chem. Phys., 33, 1059-1062.

Ising, E. (1925). Beitrag zur theorie des ferromagnetismus. Z. Phys., 31, 253-258.

Istrail, S. (2000) .Statistical mechanics, three-dimensionality and NP-completeness. I. Universality of intractability of the three-dimenaional Ising model is impossible. Proceedings of the 31st ACM Annual Symposium on the Theory of Computing, 21-23.

Jiang, W. et al. (2000). Specific heat of spin-3/2 transverse Ising model with the cyrstal field on honeycomb lattice. Phys. Stat. sol. b, 219, 157-161.

Kac, M. & Ward, J. C. (1952). A combinatorial solution of the two dimensional Ising model. Phys. Rev., 88, 1332-1337.

Kaneyoshi, T. (1993). Differential operator technique in the Ising spin systems. Acta. Phys. Polon. A, 83, 703-738.

Kaneyoshi, T. (1999). A new type of cluster theory in Ising models (I). Physica A, 269, 344-356.

Kasteleyn, P. W. (1963). Dimer statistics and phase transitions. J. Math. Phys., 4, 287-293.

Kaufman, B. (1949). Crystal Statistics. II. Partition function evaluated by spinor analysis. Phys. Rev., 76, 1232-1243.

Lou, S. L. & Wu, S. H. (2000) .Three dimensional Ising model and transfer matrices. arXiv : cond-mat/0003367.

Ma, Y. Q. & Ma, Y. G. (1993). Reentrant phase-transition and tricritical points in a quantum transverse spin system with a random field. Phys. Lett. A, 173, 373-376.

Matsudai, N. (1973). Ising ferromagnets with random impurities. J. Phys. Soc. Jpn., 35, 1593-1599.

Onsager, L.(1944). Crystal Statistics. I. A two dimenaional model with an order-disorder transition . Phys. Rev., 65, 117-149.

Peierls, R. E. (1936). Proc. Camb. Phil. Soc., 150, 552.

Potts, R. B. (1952). Some generalized order-disorder transformations. Proc. Camb. Phil. Soc., 48, 106-109.

Santos, R. R. dos (1982). J. Phys. C, 15, 3141.

Tamura, I. et al.(1984). Surface magnetism of a transverse Ising-model with a disordered surface. J. Phys C, 17, 3207-3221.

Tucker, J. W. (1994). Generalized Van der Waerden identities. J. Phys. A, 27, 659-662.

Vdovichenko, N. V. (1964) .Spontaneous magnetization of a plane dipole lattice. Soviet Physics JETP, 21, 350-352.

T.C. YÜKSEKÖĞRETİM KURULU
DOKÜMANTASYON MERKEZİ