S.Ü. Fen-Edebiyat Fakültesi Fen Dergisi Sayı 18 (2001) 1-6, KONYA

Ground and Excited State Spin Configurations of Tetragonal Lattice (Ising Model Spin 1/2)

H.Şevki DARENDELİOĞLU[1]

Abstract: *The magnetization process of tetragonal lattice has been analyzed by using the 9-sublattice model with Ising spin 1/2.The possible ground and excited state spin configurations are obtained and the stability conditions of the configurations are given in terms of linear exchange constant and third -order magnetic perturbation constant.*

Key words: **Ising Model, Spin Configuration, Exchange Constant**

Tetragonal Örgünün Taban ve Uyarılmış Spin Şekillenimleri (Ising Modeli Spin1/2)

Özet:Tetragonal örgünün manyetizasyon süreci Ising spin 1/2 li 9-altörgü modeli kullanılarak analiz edilmiştir. Mümkün olabilen taban ve uyarılmış spin şekillenimleri elde edilmiş ve bu şekillenimlerin kararlılıkları lineer değişim sabiti ve üçüncü mertebeden manyetik pertürbasyon sabiti cinsinden verilmiştir.

Anahtar Kelimeler: **Ising Model, Spin Şekillenimi, Değiş-tokuş Sabiti**

Introduction

In systems which contain magnetic ions or atoms, very different kind of ordered spin configuration of the magnetic moment may occur depending on the details of the interactions between the spins and on the qualitative and quantitative details of the system. Spin configurations corresponding to the minimum energy under some simplifying assumptions about the interaction like specified interactions between the nearest and the next-nearest neighbours and isotropic have been studied theoretically and experimentally by neutron diffraction studies. Though one can hope that the spin configurations are determined by the geometry of the system and by the range and strength of interaction however it is not an easy proplem to determine the ground state spin configuration when the range of interaction extends beyond the next nearest neighbours.

1 Selçuk University, Faculty of Sciences and Arts, Physics Dept.(42031), Konya-Turkey

The magnetization of an Ising spin antiferromagnet increases stepwise at absolute zero with increasing field strength. The Geometrical Inequalities Method (GIM) will be used in order to determine the state of lowest energy of our tetragonal Ising spin system under an external field. This method has been proposed by J. Kanamori [1] and used largely by others [2-6] .

Theory

Let us investigate the ground state spin configuration of tetragonal lattice using the 9-sublattice model with Ising spin 1/2. The nearest-neighbour spin interactions will only be considered. J and H_3 are the nearest -neighbor bilinear exchange constant and third order perturbation term respectively. The magnetic Hamiltonian appropriate to the system defined by Fig.1, in the case of Blume-Emery-Griffiths interactions [7] , is as follows:

$$H = -J\sum_{\langle ij \rangle} S_i S_j - H_3 \sum_{\langle ij \rangle} S_i S_j (S_i + S_j) - g\mu_B H \sum_i S_i$$

where J is the nearest -neighbour bilinear exchange interaction constant.
H_3 is third order magnetic perturbation.
μ_B is Bohr magneton.
H is the internal and/or external magnetic field.
The symbol $\sum_{\langle ij \rangle}$ implies that the summations are over all pairs of the nearest neighbours

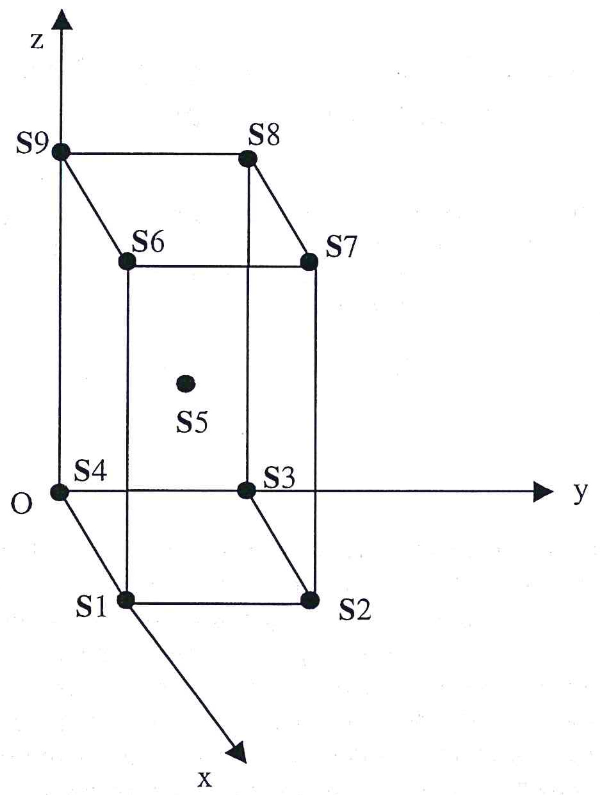

Fig. 1.Tetragonal Lattice Composed of Nine Spin 1/2 .

In a magnetic field parallel to the spin direction one may observe intermediate phases (Configurations) corresponding to the reversal of some of the down spins. If one supposes that spin flop phases do not occur, this leads to a step by step metamagnetic behaviour. At zero temperature the stable phase in a given magnetic field is that of minimum energies. The energy of the spin system is quadratic and tri form in the spin variables S each of which can take on only discrete values which for simplicity are taken as ± 1.

Description without external field

Let us take $H = 0$. If a set of values of J and H_3 are given one can obtain the exchange energies for various spin configurations. By comparing these exchange energies with each the ground state spin configurations for the set of values of J and H_3 are determined. Following this procedure two ferromagnetic and two ferrimagnetic spin configurations as a ground state spin configurations for all values of J and H_3 have been obtained. By including magnetic field, one has obtained one more intermediate state: A3. All possible eigenvectors are shown in Fig.2. Each eigenvector corresponds to a different spin configuration (or mode). Corresponding energies of these modes are tabulated in Table I. As seen all of the ground state configurations are degenerated (except for that of region II and III). The various regimes of the modes are shown in Table II. All of the possible stable spin configurations of the tetragonal lattice as a function of the exchange constants J and third order perturbation term H_3 are shown in Fig.3. As seen, in the case of the magnetic field $H = 0$, $J - H_3$ energy plane is divided into the three regions. I numerate them as I, II and III. The region I is two-fold degenerated, the region II and III are not degenerated But on the interface line $J + H_3 = 0$ and $J - H_3 = 0$ one has many states all of which are degenerated.

	S_1	S_2	S_3	S_4	S_5	S_6	S_7	S_8	S_9
$\|F_1\rangle$:	•	•	•	•	•	•	•	•	•
$\|F_2\rangle$:	o	o	o	o	o	o	•	o	o
$\|A_1\rangle$:	o	o	•	o	•	o	•	•	•
$\|A_2\rangle$:	o	•	o	•	o	•	o	•	o
$\|A_3\rangle$:	o	•	•	•	•	•	•	•	•

Fig. 2. The Schmematic Representations of 6 Types of the Ground and Excited State Spin Configuration Obtained in the Present Calculations.(The Signs o and • Denote Down and Up Spins Respectively.)

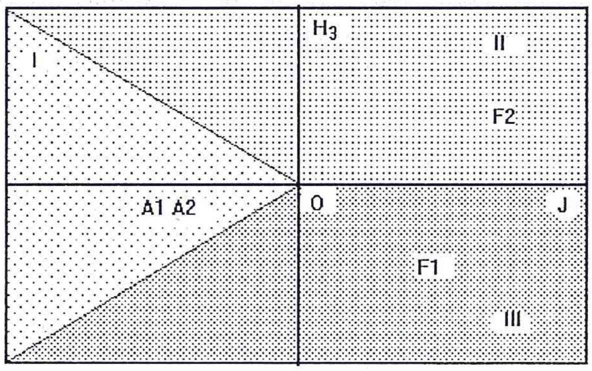

Fig. 3. Stable Spin Configuration of the Tetragonal Lattice as a Function of the J and H_3

Effect of an Applied Field on the Magnetic Behaviour of the System

When an external magnetic field is applied each Ising spin can change its direction and so new configurations can appear. At very high magnetic fields all of the spins have same direction. This is ferromagnetic configuration. However at intermediate magnetic field values some parts of spins will turn their directions. Competition between exchange energy and the Zeeman Energy determines the stable configuration. Because of this fact it is possible to obtain all type of possible spin configurations by increasing the external magnetic field for fixed values of the exchange constants J and H_3 . The magnetization process for each of the three regions have been calculated by comparing the total energy in the case $H \neq 0$. After a slightly long calculation the spin-flip type magnetization process has been found to be possible in the following three regions of the two dimensional exchange constant -perturbation parameter space.

In the region I at the beginning there are two degenerated states as seen at Fig.2. When an external magnetic field is applied and gradually increased, firstly the state A1 transforms into the state A2 at the first critical value H_{C1} (I) of the magnetic field and then the state A2 transforms into the state A3 at the second critical field value H_{C2}(I) and finally the state A3 transforms into the state F2 at the third critical field value H_{C3}(I). The value of H_{C1}(I) =12J. The value of H_{C2} (I) and H_{C3} (I) are $-2.66J - 2.66H_3$ and $-4J - 4H_3$ respectively. For this region one has the following stability condition: $J < 0$; $J - H_3 > 0$ or $J + H_3 < 0$.

Table I. Stable Spin Configurations and Corresponding Exchange Energies.

Configurations	States	Energy
Ferromagnetic	F1	$H = -12\,J + 24\,H_3$
Ferrimagnetic	F2	$H = -12\,J - 24\,H_3$
Ferrimagnetic	A1	$H = -12\,J$
Ferrimagnetic	A2	$H = 12\,J$

5) **Table II.** Stable Spin Configurations and Their Regimes.

Configurations	States	Stability Conditions
Ferromagnetic	F1	$H_3 < 0$; $J - H_3 < 0$
Ferrimagnetic	F2	$J > 0$; $H_3 > 0$; $J + H_3 > 0$
Ferrimagnetic	A1, A2	$J < 0$; $J - H_3 > 0$ or $J + H_3 < 0$

In the region II (See Fig. 3) for the regim $J > 0$ and $J + H_3 > 0$; There is a just F2 state as a only possible ground state. The system is already in the ferromagnetic state . So there is no transition field.

Finally in the region III when there is no external field one has the F1 state in which all spins are down. For the stability condition for this regime one has $H_3 < 0$ and $J - H_3 < 0$.

As one applies an external magnetic field the state F1 transforms into the state F2 immeadiately. The value of the critical field is independent of J and H_3 values. This is the only region whose critical field is independent of the exchange constants. This state is not quantizied, it continously receives energy. Corresponding values of critical fields and magnetization processes are summarized in Table III.

6) **Table III.** Critical Magnetic Fields in Terms of J and H_3

Critical Fields / Domains	H_{c1}	H_{c2}	H_{c3}
Domain I	2J	$-2.66J - 2.66H_3$	$-4J - 4H_3$
Domain II	—	—	—
Domain III	$-2.66H_3$	—	—

Results and Discussions

In this work, The ground state and excited spin configurations of tetragonal lattice using the 9 -sublattice model with Ising type spin 1/2 assuming two kinds of the interactions, bilinear exchange interactions and third order perturbation term. However the present calculation is restricted to only special type of the nearest spin interactions and further interaction will be always needed to draw more definite conclusion.

The magnetization values have been calculated and the spin configurations of the states in each process for all positive and negative values of J and H_3 . The five type of the ground and excited state spin configurations have been found to be possible for various sets of the values of the interaction parameters.

In domain III , I find that the value of the transition field H_C(III) from the configuration F1 to the configuration F2 depends on the perturbation term H_3 and is independent of J . This conclusion is indeed very interesting.

From the values of the first or second transition field for the domains, it is possible to determinate the values of the exchange constant J and H_3 For the exchange constants of the other domains, one needs of an extra data like heat capacity or susceptibility.

One observes that there is no rigid configurations; i.e. configurations with the same orientation for all ground states.

References

1- Junjiro Kanamori , **Magnetization Process in an Ising Spin System** Prog. Theor. Phys. 35 16-35 (1966)

2- Makoto Kaburagi and Junjiro Kanamori, **Ordered Structures of Adatoms in the Extended Range Lattice Gas Model** J,Appl. Phys. Suppl.2.Pt.2 145-148 (1974)

3- Makoto Kaburagi and Junjiro Kanamori, **A Method of Determining the Ground State of the Extended-Range Classical Lattice Gas Model**,Prog. Theor. Phys. 54 30-44 (1975)

4- I. Kimura, **Crystalline Field Effects.....I**, Bulletin of Fukuoka University of Education Vol. 34 Part III 27-32 (1985)

5- I. Kimura, **Crystalline Field Effects.....II,** Bulletin of Fukuoka University of Education Vol. 37 Part III 49-54 (1988)

6- I. Kimura, **Magnetic Structure and Exchange Interaction in $DyCu_2$** Journal of Magnetism and Magnetic Materials 70 273-274 (1987)

7- M. Blume,V.J. Emery and R.B. Griffiths, Phys. Rev. A 4 1071- (1971)