Vol 11 No 8, August 2002
1009-1963/2002/11(08)/0823-04

Chinese Physics

© 2002 Chin. Phys. Soc.
and IOP Publishing Ltd

# Properties of the ground state in a spin-2 transverse Ising model with the presence of a crystal field*

Jiang Wei(姜 伟)[a)b)], Wei Guo-Zhu(魏国柱)[b)],
Du An(杜 安)[b)], and Zhang Qi(张 起)[b)]

[a)] *College of Sciences, Shenyang University of Technology, Shenyang* 110023, *China*

[b)] *College of Sciences, Northeastern University, Shenyang* 110006, *China*

(Received 8 March 2002; revised manuscript received 3 April 2002)

The properties of the ground state in the spin-2 transverse Ising model with the presence of a crystal field are studied by using the effective-field theory with correlations. The longitudinal and transverse magnetizations, the phase diagram and the internal energy in the ground state are given numerically for a honeycomb lattice ($z$=3).

**Keywords:** Ising model, ground state, crystal field, magnetizations, internal energy
**PACC:** 7510H, 7510D, 7550G

## 1. Introduction

Ising models and their many variations have been one of the most actively studied systems in statistical mechanics,[1−5] because they are useful for studying a great variety of physical systems, such as pure and disordered magnetic systems as well as special magnetic materials (or molecular-based magnetic materials, surface and multilayers). They have been widely investigated by various techniques: molecular field approximation,[6] linear chain approximation,[7] cluster variational method in pair approximation,[8] the renormalization group technique,[9] etc. Many theoretical works have been studied by the effective-field theory with correlations, such as the effects of a transverse field or a crystal field interaction on the transition temperature and magnetic properties of the systems.[10,11] On the other hand, Liu *et al*[12] have discussed nonlinear magnetization dynamics of a classical ferromagnet with anisotropies in an external magnetic field. However, the properties of an Ising model interacting with both the transverse field and the crystal field have not been reported in previous works. In Ref.[13], the phase diagrams of a single spin-1 Ising system with a single-ion anisotropy in a transverse field have been examined. Jiang *et al*[13] have given the general expressions of the second-order transition and tricritical point for a general coordination number. It is important that this model be extended to higher spin values. As far as we know, there has not been an investigation of the ground-state properties concerning the spin-2 transverse Ising model with the presence of a crystal field. Therefore, this is the aim of this paper. In section 2, the basic framework for the spin-2 transverse Ising model with the presence of a crystal field is given. The numerical results and discussions are presented in section 3, and section 4 contains the conclusion.

## 2. Theory

The following Hamiltonian describes the spin-2 transverse Ising model interacting with a crystal field

$$H = -J \sum_{<i,j>} S_i^z S_j^z - \Omega \sum_i S_i^x - D \sum_i (S_i^z)^2, \quad (1)$$

where $S_i^z$ and $S_i^x$ are components of a spin-2 operator at site $i$, $J$ is the exchange interaction constant, $D$ is the crystal field and $\Omega$ represents the transverse field. The first summation is taken over all the nearest-neighbour pairs.

As given in Ref.[14], within the effective-field theory and differential operator technique, the longitudinal and transverse magnetizations are given by

$$M_z \equiv < S_i^z > = \left[ \cosh(J\eta\nabla) + \frac{M_z}{\eta} \sinh(J\eta\nabla) \right]^3 F(x)|_{x=0}, \quad (2)$$

*Project supported by the Foundation for the Key Program of Science and Technology Research from Chinese Ministry of Education (Grant No 99026)

$$M_x \equiv < S_i^x > = \left[\cosh(J\eta\nabla) + \frac{M_z}{\eta}\sinh(J\eta\nabla)\right]^3 H(x)|_{x=0}, \quad (3)$$

$$\eta^2 \equiv < S_i^z > = \left[\cosh(J\eta\nabla) + \frac{M_z}{\eta}\sinh(J\eta\nabla)\right]^3 G(x)|_{x=0}, \quad (4)$$

where $\nabla = \partial/\partial x$ is a differential operator. The functions $F(x)$, $H(x)$ and $G(x)$ can be, respectively, described as

$$F(x) = \frac{1}{\sum_{n=1}^{5}\exp(\beta\lambda_n)}\left\{\sum_{n=1}^{5}\langle\varphi_n|S_i^z|\varphi_n\rangle\exp(\beta\lambda_n)\right\}, \quad (5)$$

$$H(x) = \frac{1}{\sum_{n=1}^{5}\exp(\beta\lambda_n)}\left\{\sum_{n=1}^{5}\langle\varphi_n|S_i^x|\varphi_n\rangle\exp(\beta\lambda_n)\right\}, \quad (6)$$

$$G(x) = \frac{1}{\sum_{n=1}^{5}\exp(\beta\lambda_n)}\left\{\sum_{n=1}^{5}\langle\varphi_n|(S_i^z)^2|\varphi_n\rangle\exp(\beta\lambda_n)\right\}. \quad (7)$$

Here, $\lambda_n$ ($n$=1,2,3,4,5) is the eigenvalue and $\varphi_n$ represents the eigenfunction with the eigenvalue $\lambda_n$ of $-H_i$ (which includes all parts of $H$ associated with site $i$)

In order to determine the phase transition point of the system, we must expand the right-hand side of Eqs.(5), (6) and (7). The following equations are thus obtained

$$M_z = A_1 M_z + A_2 M_z^3, \quad (8)$$

$$M_x = B_1 + B_2 M_z^2, \quad (9)$$

$$\eta^2 = q_0 + q_1 M_z^2. \quad (10)$$

where

$$A_1 = \frac{3}{4\eta}[F(3J\eta) + F(J\eta)],$$
$$A_2 = \frac{1}{4\eta^3}[F(3J\eta) - 3F(J\eta)], \quad (11)$$

$$B_1 = \frac{1}{4}[H(3J\eta) + 3H(J\eta)],$$
$$B_2 = \frac{3}{4\eta^2}[H(3J\eta) - H(J\eta)], \quad (12)$$

$$q_0 = \frac{1}{4}[G(3J\eta) + 3G(J\eta)],$$
$$q_1 = \frac{3}{4\eta^2}[G(3J\eta) - G(J\eta)]. \quad (13)$$

The coefficients $A_1, A_2, B_1, B_2, q_0$ and $q_1$ can be easily calculated by using the mathematical relation $e^{\alpha\nabla}f(x) = f(x+\alpha)$.

In the vicinity of the second-order transition line, the magnetization $M_z$ can be written as

$$M_z^2 = \frac{1-a}{b}, \quad (14)$$

where

$$a = A_1, \quad (15)$$

$$b = \frac{A_1' B_1}{2\eta_0 - q_0'} + A_2. \quad (16)$$

When $a$=1 and $b < 0$, the transition is of second order; but when $a$=1 and $b > 0$ the transition is of first order. The tricritical point at which the phase transition changes from the second order to the first order is determined by $a$=1 and $b$=0. The coefficients $A_1'$ and $q_0'$ are the first derivative of $A_1$ and $q_0$ with $\eta_0$, which is the value of $\eta$ at $T = T_c$.

The internal energy of the system can be obtained from the thermodynamical average of the Hamiltonian and the internal energy per site is

$$\frac{U}{N} = -\frac{1}{2} < E_i S_i^z > -\Omega < S_i^x > -D < (S_i^z)^2 >, \quad (17)$$

where $N$ is the total number of magnetic atoms. Within the above framework, we can investigate the properties of the ground state ($T$=0K, $\beta \to \infty$) for a honeycomb lattice system.

## 3. Numerical results and discussion

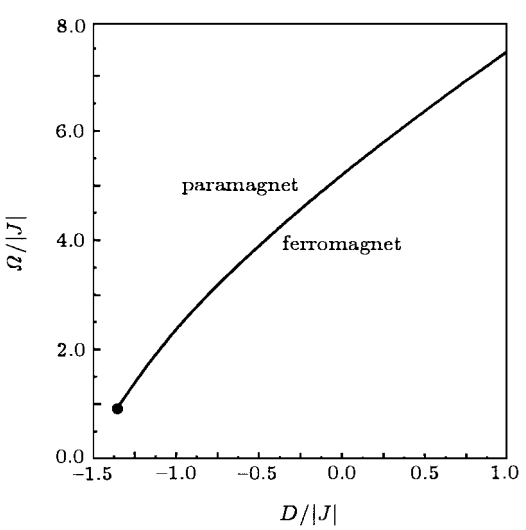



**Fig.1.** Phase diagram of the ground state for the honeycomb lattice in the $(\Omega/|J|, D/|J|)$ plane. The black dot denotes the tricritical point.

Figure 1 shows the phase diagram of the ground state in the $\Omega/|J| - D/|J|$ plane for the honeycomb lattice. From the figure we can see that the curve separates the $\Omega/|J| - D/|J|$ plane into two regions: one is the ferromagnetic phase region, and the other is the paramagnetic phase region. For this system we can find the tricritical point at which the phase transition changes from second order to first order. The black dot denotes the tricritical point at $D_t/|J| = -1.3466$ and $\Omega_t/|J| = 0.9610$, which is obtained in the present study.

The crystal field $D$ dependence of the longitudinal and transverse magnetizations for the honeycomb lattice in the ground state are given in Figs.2(a) and 2(b), when the transverse field is selected at some typical values. From Fig.2(a) we see that the value of $M_z$ decreases with increasing transverse field $\Omega$ when $D$ is fixed. From Fig.2(b), we see that $M_x$ increases with increasing transverse field $\Omega$ when $D$ is fixed.

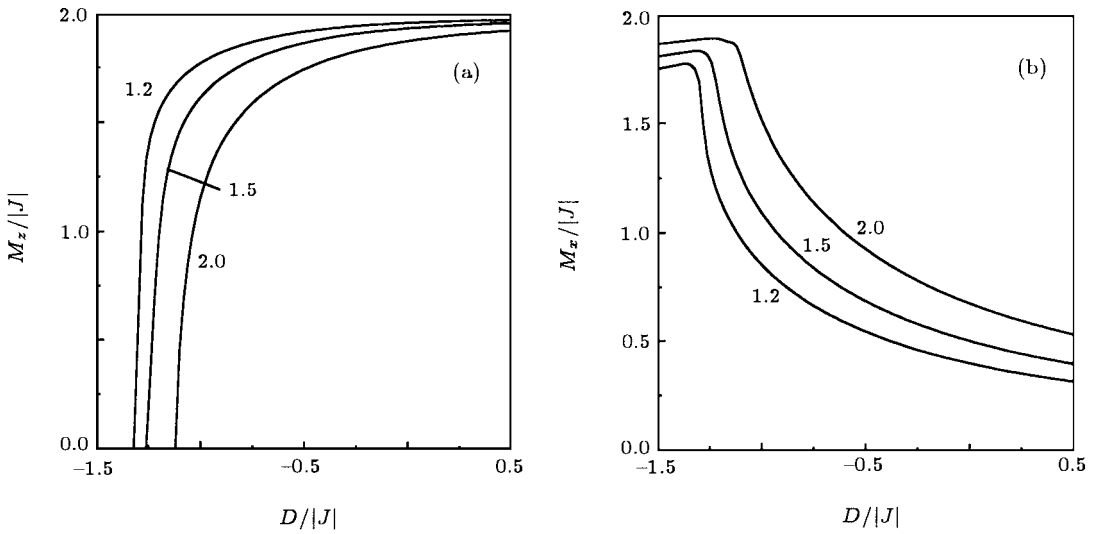



**Fig.2.** The crystal field $D$ dependence of magnetization: (a) longitudinal magnetization $M_z$; (b) transverse magnetization $M_x$. The numbers at the curves are for $\Omega/|J|$.

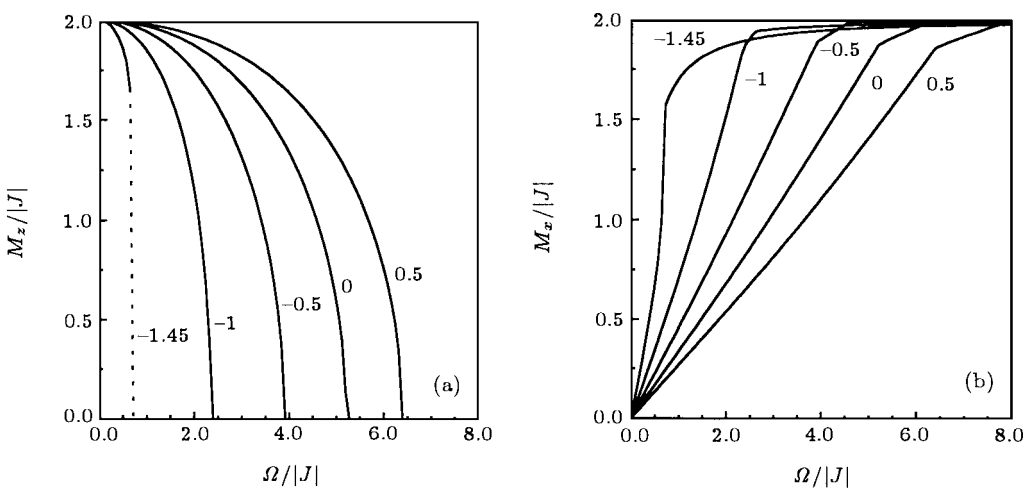



**Fig.3.** The transverse field $\Omega$ dependence of magnetization for honeycomb lattice in the ground state: (a) the longitudinal magnetization $M_z$; (b) the transverse magnetization $M_x$. The numbers at the curves are for the crystal field $D/|J|$.

In Fig.3(a) and 3(b) we show the transverse field $\Omega$ dependences of the longitudinal and transverse magnetizations for the honeycomb lattice in the ground state, when the crystal field $D$ is selected at some typical values. From Fig.3(a), we know that the longitudinal magnetization $M_z$ decreases with the increase of $\Omega$ when $D$ is fixed. The dashed line represents the first-order phase transition. In Fig.3(b), the

$M_x$ curves increase linearly with $\Omega$ and change their inclination at the transition points. As seen from these figures, transverse magnetizations are always given by $M_x$=0, and the values of $M_z$ are 2.0 when $\Omega$=0. When $\Omega$ increases from zero, each curve of $M_z$ falls from its saturated value and reaches zero, while each curve of $M_x$ increases from zero to its value for spin-2.

Finally, in Figs.4(a) and 4(b) we plot the variation of ground-state energy $U$ with $D$ and $\Omega$ for honeycomb lattice. As far as we know, these quantities (for spin-2) have not been reported in the literature. From Fig.4(a), we see that the ground-state energy curves are continuous at the transition points. We can also see that the ground-state energy increases linearly with decreasing $D$ and changes the inclination at the transition point. Figure 4(b) shows that the ground-state energy decreases with the increase of $\Omega$ when $D$ is fixed.

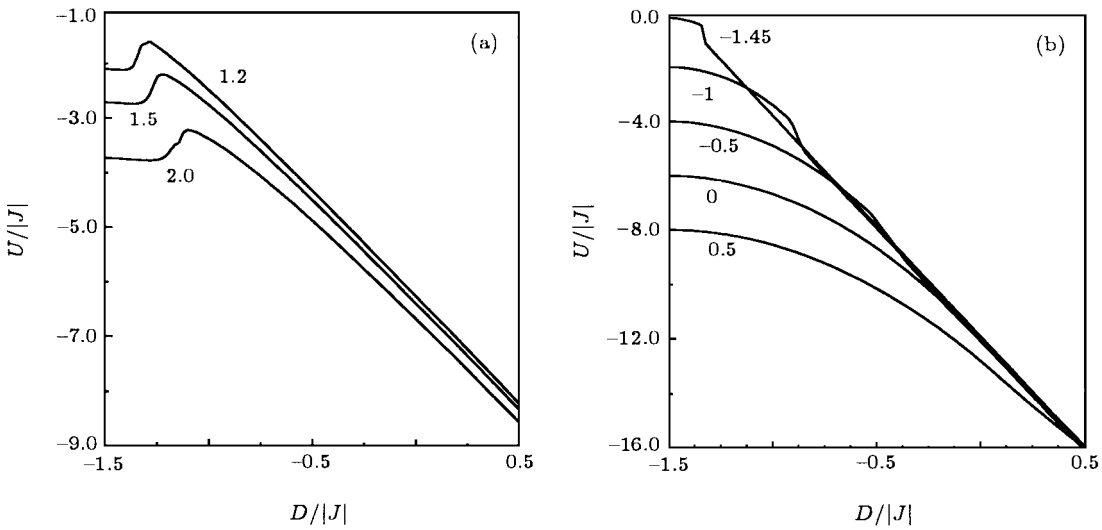



**Fig.4.** (a) The crystal field $D$ dependence of internal energy $U$. The numbers at the curves are the values of $\Omega/|J|$. (b) The transverse field $\Omega$ dependence of the internal energy $U$. The numbers at the curves are the values of $D/|J|$.

## 4. Conclusion

In this paper we have investigated the ground-state properties for the spin-2 transverse Ising model system with the presence of a crystal field by using the effective-field theory with correlations. The phase diagram has been calculated for the honeycomb lattice in the ground state. We have provided the equations for calculating the transverse and longitudinal magnetizations and the internal energy. As discussed in section 3, a number of interesting phenomena of the ground state have been found, which are due to the transverse magnetic field and the crystal field. For the model with spin-2, we find that tricritical behaviour does exit. We hope that these results will be potentially useful for experimental research.

## References

[1] Gao Z, Wang Z L and Xu J H 1997 *Acta Phys. Sin.* **46** 2029 (in Chinese)
[2] Shao Y Z, Lan T and Lin G M 2001 *Acta Phys. Sin.* **50** 942 (in Chinese)
[3] Laabo M, Saber A, Benab M and Kerou 1999 *Chin. Phys.* **8** 199
[4] Ni J and Gu B L 2000 *Chin. Phys.* **9** 469
[5] Deng L L and Yan S L 2002 *Chin. Phys.* **11** 4
[6] Kaufman M and Kanner M 1990 *Phys. Rev.* B **42** 2378
[7] Chakraborty K G and Tucker J W 1986 *Physica* A **137** 111
[8] Ng W M and Barry J H 1978 *Phys. Rev.* B **17** 3675
[9] Dickinson H and Yeomans J 1983 *J. Phys. C: Solid State Phys.* **16** L345
[10] Kaneyoshi T, Jascur M and Fittipaldi I P 1993 *Phys. Rev.* B **48** 250
[11] Xin Z H, Wei G Z and Liu T S 1998 *Physica* A **248** 442
[12] Liu W M, Wang X B, Pu F C and Huang N N 1996 *Phys. Rev.* E **54** 4612
Liu W M, Wang X B, Pu F C and Huang N N 1999 *Phys. Rev.* B **60** 12893
[13] Jiang, X F, Li Z Y, Zhong J L and Yang C Z 1993 *Phys. Rev.* B **47** 827
[14] Jiang W, Wei G Z and Xin Z H 2001 *Physica* A **284** 215