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Equilibrium behavior of the mixed spin-1 and spin-3/2 ising system by using the lowest approximation of the cluster variation method

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We have studied equilibrium behavior of the mixed spin-1 and spin-3/2 Ising system in the absence and presence of an external magnetic field by using the lowest approximation of the cluster-variation method. We have obtained the thermal variation of the stable, dipole and quadrupolar moment order paramaters for several of coupling parameters, D/J.Some outstanding features are found in the temperature dependences of the order parameters. The phase transitions of the stable branch of the order paramaters are investiated extensively. Then we have presented stable phase diagrams of the mixed spin-1 and spin-3/2 Ising system.

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1. Introduction

Over recent years, mixed spin systems have become one of the most actively studied topics in statistical physics and condensed matter physics due to the reason that they provide simple but interesting models to investigate molecular magnetic materials in which are considered to be possible useful materials for magneto-optical recording [1-4]. The spin-1 and spin-3/2 mixed system is the one of the most extensively studied mixed Ising systems after the mixed spin-1/2 and spin-1 system. The equilibrium properties of the mixed spin-1 and spin-3/2 Ising system were examined by various methods such as the effective-field theory (EFT) [5], mean-field approximation (MFA) based on Bogoliubov inequality for the Gibbs free energy [6], the cluster variation method with the pair approximation (CVMPA) [7], the Monte Carlo simulations (MC) [8]. The exact formulation of the mixed spin-1 and spin-3/2 Ising ferrimagnetic systems on the Bethe lattice using the exact recursion equations was given in detail [9]. Recently, the dynamic phase transitions are studied, within a mean-field approach, in the kinetic mixed spin-1 and spin-3/2 Ising system under the presence of a time varying (sinusoidal) magnetic field by using the Glauber-type stochastic dynamics [10]. The dynamic phase transition points are obtained and the phase diagrams are presented in three different planes.

In spite of these studies, the equilibrium properties of the mixed spin-1 and spin-3/2 Ising system in the absence and the presence of an external magnetic field is not investigated using the lowest approximation of the cluster-variation method (LACVM). The influence of an external magnetic field is also investigated. The LACVM, in spite of its simplicity and limitations such as the correlations of spin fluctuations have not been considered, is an adequate starting point in which with in this theoretical framework it is easy to determine the complete phase diagrams and find some outstanding features in the temperature dependences of the order parameters.

The organization of the remaining part of this paper is as follows. In Section 2, we defined the model briefly and obtain its solutions at equilibrium within the LACVM. The thermal variations of the order parameters are investigated in Section 3. In Section 4, the phase diagram of the system is obtained for the absence and the presence of an external magnetic field, respectively. Finally, we give a summary and conclusion in Section 5.

2. The model and method

The mixed spin-1 and spin-3/2 Blume-Capel Ising system consists of two interpenetrating sublattices. The sites of one sublattice, called sublattice A, have spins $\sigma = \pm 1$ and, 0 and the sites of the other sublattice, called sublattice B, have spins $S = \pm 1/2$ and $\pm 3/2$. Each spin σ has only S-spins as nearest neighbors and vice versa. The average value of each the spin states will be denoted by X_1^A, X_2^A and X_3^A on the sites of sublattice *A* and X_1^B, X_2^B, X_3^B and X_4^B on sublattice *B*, which are also called the state or point variables. These variables obey the following two normalization relations for *A* and *B* sublattices:

$$\sum_{i=1}^{3} X_i^{\,A} = 1 \quad \text{and} \quad \sum_{j=1}^{4} X_j^{\,B} = 1 \tag{1}$$

In order to account for the possible two-sublattice structure we need five long-range order parameters which are introduced as follows:

$$M_A \equiv \left\langle \sigma_i^A \right\rangle, \quad Q_A = 2\left\langle \left(\sigma_i^A\right)^2 \right\rangle - 2\,, \; M_B \equiv \left\langle S_j^{\,B} \right\rangle,$$

$$Q_B \equiv \left\langle (S_j^{\,B})^2 \right\rangle - \frac{5}{4} \text{ and } R_B \equiv \frac{5}{3}\left\langle (S_j^{\,B})^3 \right\rangle - \frac{41}{12}\left\langle S_j^{\,B} \right\rangle, \tag{2}$$

for A and B sublattices, respectively. M_A and M_B are the average magnetizations which are the excess of the one orientation over the other, called magnetizations; Q_A and Q_B are the quadrupolar moments which are the average squared magnetizations; and R_B is the octupolor-order parameters. The phase regions, i.e. disordered, ferrimagnetic with its cofigurations, antiferrimagnetic with its cofigurations and antiquadrupolar or staggered phase with $m_A = m_B = 0$, $q_A \neq q_B \neq 0$, are indicated with (D), F(σ, S), AF(σ, S) and (A) respectively.

The order parameters can be expressed in terms of the internal variables and are given by

$$M_A = X_1^A - X_3^A, \quad M_B = \frac{1}{2}[3X_1^B + X_2^B - X_3^B - 3X_4^B],$$
$$Q_A = X_1^A + X_2^A, \quad Q_B = X_1^B - X_2^B - X_3^B + X_4^B$$
$$R_B = \frac{1}{2}(X_1^B - X_4^B) + \frac{3}{2}(X_3^B - X_2^B) \tag{3}$$

Using Eqs. (1) and (3), the internal variables can be expressed as a linear combinations of the order parameters:

$$X_1^A = \frac{1}{2}(M_A + Q_A), \quad X_2^A = 1 - Q_A, \quad X_3^A = \frac{1}{2}(Q_A - M_A),$$
$$X_1^B = \frac{1}{4}(1 + Q_B) + \frac{1}{10}(3M_B + R_B), \quad X_2^B = \frac{1}{4}(1 - Q_B) + \frac{1}{10}(M_B - 3R_B), \quad X_3^B = \frac{1}{10}(3R_B - M_B) + \frac{1}{4}(1 - Q_B) \text{ and}$$
$$X_4^B = \frac{1}{4}(1 + Q_B) - \frac{1}{10}(3M_B + R_B). \tag{4}$$

The mixed spin-1 and spin-3/2 Ising model Hamiltonian with the bilinear (J) nearest-neighbor pair interaction and a single-ion potential or crystal field interaction (D) in the presence of an external magnetic field is given by

$$\mathbf{H} = -J\sum_{\langle i,j\rangle}\sigma^A_i S^B_j + D\Big(\sum_i[2(\sigma_i^A)^2 - 2] + \sum_j[(S^B_j)^2 - 4/5]\Big) - H\Big(\sum_i \sigma_i^A + \sum_j S_j^B\Big), \tag{5}$$

where <*ij*> indicates a summation over all pair of nearest-neighboring sites .

The equilibrium properties of the system are determined by the lowest approximation of the cluster variation method (LACVM) which is identical to the mean-field approximation. The method consists of the following there steps: (i) consider a collection of weakly interacting systems and define the internal variables, (ii) obtain the weight factor in terms of the internal variables, (iii) find the free energy expression and minimize it.

The weight factors W^A and W^B can be expressed in terms of the internal variables for the *A* and *B* sublattices , respectively as;

$$W^A = \frac{N^A!}{\prod_{i=1}^{3}(X_i^A N^A)!} \quad \text{and} \quad W^B = \frac{N^B!}{\prod_{j=1}^{4}(X_j^B N^B)!} \tag{6}$$

where N^A and N^B are the number of lattice points on the *A* and *B* sublattices respectively. *A* simple expression for internal energy of the system is found by working out Eq.(5) in the lowest approximation of the cluster variation method. This leads to

$$\frac{E}{N} = -JM_AM_B + D(Q_A + Q_B) - H(M_A + M_B) \tag{7}$$

Substituting Eq.(3) in to (7) the internal energy per site can be written as

$$\frac{E}{N} = -J\{(X_1^A - X_3^A)[\frac{1}{2}(3X_1^B + X_2^B - X_3^B - 3X_4^B)]\} + D[(X_1^A + X_3^A) + (X_1^B - X_2^B - X_3^B + X_4^B)] - H\{(X_1^A - X_3^A) + [\frac{1}{2}(3X_1^B + X_2^B - X_3^B - 3X_4^B)]\} \tag{8}$$

where $N = N^A + N^B$ is the total lattice points.

Using the definition of the entropy S_e($S_e = k \ln W$) with the Stirling approximation, the free energy *F* (*F=E-TS*) per site can now be found as

$$f = \frac{F}{N} = -JM_AM_B + D(Q_A + Q_B) - H(M_A + M_B) + \frac{1}{\beta}\{\sum_{i=1}^{3}X_i^A \ln X_i^A + \sum_{j=1}^{4}X_j^B \ln X_j^B\} + \beta\lambda^A\{1 - \sum_{i=1}^{3}X_i^A\} + \beta\lambda^B\{1 - \sum_{j=1}^{4}X_j^B\} \tag{9}$$

where λ^A and λ^B are introduced to maintain the normalization condition, $\beta = 1/kT$, *T* is the absolute temperature and k is the Boltzmann factor. The minimization of Eq.(9) with respect to X_i^A and X_j^B and using Eq.(3), the self-consisting equations are found to be

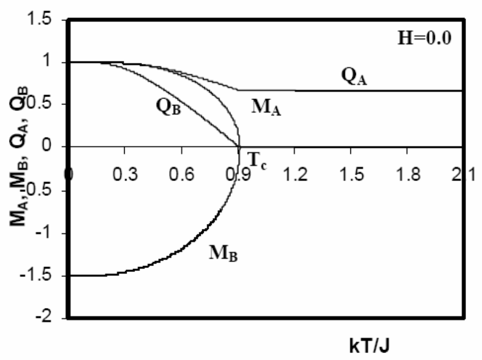
$$M_A = \frac{2Sinh[\beta(JM_B + H)]}{2Cosh[\beta(JM_B + H)] + e^{\beta D}},$$
$$M_B = \frac{3e^{-\beta D}Sinh[\frac{3}{2}\beta(JM_A + H)] + e^{\beta D}Sinh[\frac{1}{2}\beta(JM_A + H)]}{2e^{-\beta D}Cosh[\frac{3}{2}\beta(JM_A + H)] + 2e^{\beta D}Cosh[\frac{1}{2}\beta(JM_A + H)]},$$
$$Q_A = \frac{2Cosh[\beta(JM_B + H)]}{2Cosh[\beta(JM_B + H)] + e^{\beta D}},$$
$$Q_B = \frac{2e^{-\beta D}Cosh[\frac{3}{2}\beta(JM_A + H)] - 2e^{\beta D}Cosh[\frac{1}{2}\beta(JM_A + H)]}{2e^{-\beta D}Cosh[\frac{3}{2}\beta(JM_A + H)] + 2e^{\beta D}Cosh[\frac{1}{2}\beta(JM_A + H)]} \tag{10}$$

In this point, we should mention that since the behavior of R_B are similar to the M_B, we will not obtained R_B and investigate their behaviors as many researches have made. We are now able to examine the thermal behavior of the order parameters of the mixed spin-1 and spin-3/2 Ising model in an external field by solving the self-consistent equations, i.e.,(10), numerically. In the following section, we shall examine the thermal variation of the systems.

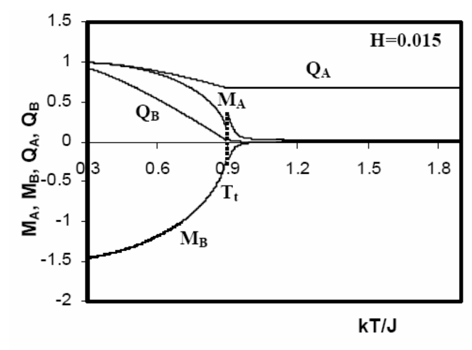
3. Thermal variations

In this section, we investigate the temperature dependence of the order parameters in the absence and presence of an external magnetic field by solving these four non-linear algebraic equations, namely, the set of self-consistent equation, i.e., Eq. (10), numerically. These equations are solved by using the Newton-Raphson method and the thermal variations of M_A, M_B, Q_A and Q_B for several of coupling parameters, D/J, are plotted in Fig.1(a) for H=0.0 and Fig. 1(b).for H≠0. In Figs, solid lines indicate the stable solutions. In the figures, T_c, $T_{c'}$ and T_t are the critical or the second-order phase transition (also called Neel temperature) and the first-order phase transition temperatures, respectively. T_{cm} and T_{cq} represent the critical or the second-order phase transition temperatures for only the sublattice magnetizations and quadrupolar order parameters, respectively. This classification is done by comparing the free energy values of these solutions and as well as investigating to the free energy surfaces. First, we will investigate the thermal variations of the sublattice magnetizations and quadrupolar order parameters in the absence and presence of an external magnetic field. The system exhibits the following two different topological types of thermal behaviors, seen in Figs. 1(a)-(c).

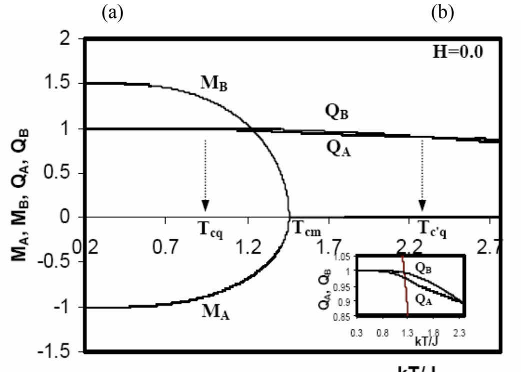
a) *Type 1*: The thermal variations of M_A, M_B, Q_A and Q_B are represented in Fig.1(a).The stable branches of magnetizations of M_A, M_B and the stable branches of the quadrupolar order parameter of Q_B decrease to zero continuously as the temperature increases; therefore a second-order phase transition occurs in M_A, M_B and Q_A .That is, for M_A=1.0, $M_B=-\frac{3}{2}$ and $Q_A = Q_B$ =1.0 at zero temperature, this type corresponds to the antiferrimagnetic phase. As the temperature increases, M_A decreases and M_B increases continuously and they meet at kT/J =0.937 which is T_c , hence a second-order phase transition occurs. The stable branch of quadrupolar order parameter, Q_A, for the B sublattice, decreases until T_c , as the temperature increases and makes a cusp at T_c (0.937) and then Q_A becomes 0,666.



(a)



(b)



(c)

Fig. 1. Thermal variations of the order parameters, M_A, M_B ,Q_A and Q_B . In the figures, T_c, $T_{c'}$ and T_t are the critical or the second-order phase transition (also called Neel temperature) and the first-order phase transition temperatures, respectively. T_{cm} and T_{cq} represent the critical or the second-order phase transition temperatures for only the sublattice magnetizations and quadrupolar order parameters, respectively.(a) Exhibiting a second-order phase transition for only the sublattice magnetizations, J=-1.00, D=0.00 and H=0.00. (b) Exhibiting two successive phase transitions in which the first one is a first-order and the second one is a second-order phase transition for the order parameters, J=-1.00, D=0.00 and H=0.015. (c) Same as (a), but D=-3.40.

On the other hand, thermal variations of the order parameters in the presence of an external magnetic field are shown in Fig. 1(b). In this case, the system undergoes two phase transitions in which the first one is a first-order phase transition from the antiferrimagnetic to the antiferromagnetic phase and the second one is a second-order phase transition from the antiferromagnetic phase to the disordered phase, seen in Fig. 1(b).

b) *Type 2*: For M_A=-1.0, M_B=1.0 and $Q_A = Q_B$=1.0 at zero temperature. As the temperature increases, M_A increases and M_B decreases continuously and they meet at kT/J =1.491 which is T_c, hence a second-order phase transition occurs. In addition to the quadrupolar order parameters, namely Q_A and Q_B, undergo successive two second-order phase transitions at two different temperatures, i.e., T_c=0.693 and $T_{c'}$ = 2.381 , seen in Fig. 1 (c). The antiquadrupolar or staggered phase transition with $M_A=M_B$=0.0 and $Q_A \neq Q_B \neq 1.0$ between kT/J=0.693 and kT/J=2.381 occurs. This fact is seen explicitly inset figure in the Fig.1 (c).

4. Phase diagrams

We can now present the phase diagrams of the system in this section. The critical or second-order phase transition temperatures for the sublattice order parameters in the case of a second-order phase transition are calculated numerically. The first –order phase transition temperatures for the stable branch of the order parameters are found by using the free energy values while increasing and decreasing the temperature. The temperature at which the free energy values equal to each other is the first –order phase transition temperatures, T_t . In these figures the solid curves denote the second-order phase transition, the dashed curves denote the first-order phase transition and special points are the tricritical (T) for the stable branches of the order parameters, respectively, seen Fig.2. Fig.3(a)-(b) show the phase diagrams in the (D/J, kT/J) plane with different D/J values.

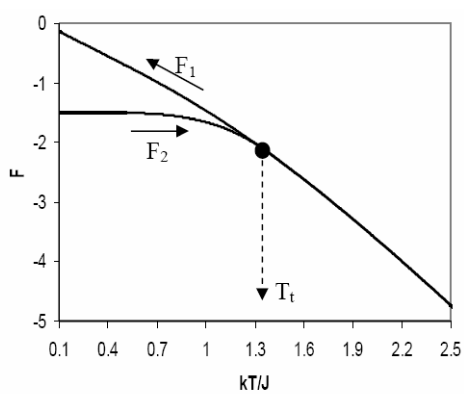
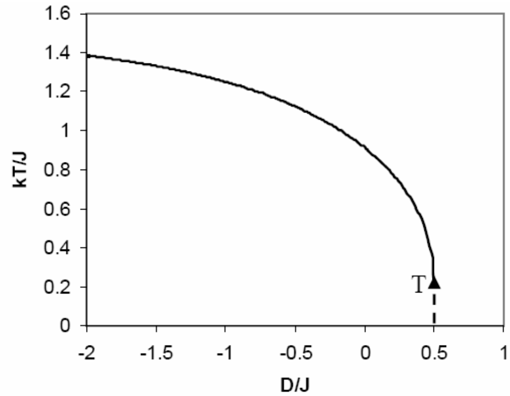


Fig. 2. Free energy as a function of temperature, J=-1.0, H=0.00. F_1 corresponds to free energy values while decreasing the temperature (arrow 1)and F_2 corresponds to free energy values while increasing of temperatures (arrow 2). The temperature where both free energies equal to each other is the first-order phase transition temperature, T_t, for order parameters, marked with a filled circle.



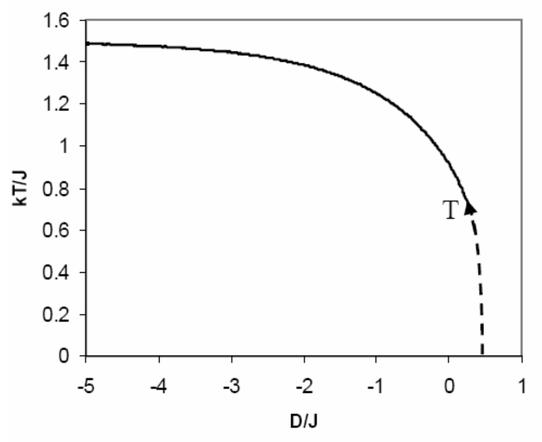


Fig. 3. Phase diagrams of the Mixed Spin-1 and Spin-3/2 Isıng system in the (D/J, kT/J) plane. In these figures the solid curves denote the second-order phase transition, the dashed curves denote the first-order phase transition and special points are the tricritical (T).

5. Summary and conclusion

In this work, we have investigated the temperature dependence of the order parameters of the mixed spin-1 and spin-3/2 Ising system in the absence and the presence of an external magnetic field by the LACVM. We presented the equilibrium phase diagram for the absence and the presence of an external magnetic field, respectively. The influence of an external magnetic field is also examined.

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