STUDY OF FERRIMAGNETIC MIXED SPIN-3/2 AND SPIN-5/2 SYSTEM USING ISING MODEL

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Abstract

The mixed spin-3/2 and spin-5/2 Ising ferrimagnetic system with different anisotropies has been investigated using the mean field approximation (MFA) .The phase diagram of the system has also been discussed in the anisotropy dependence of transition temperature. It is found that a reentrant ferrimagnetic phenomenon in the ordered system depends strongly on the anisotropy of the mixture.

دراسة نظام فيري مغناطيسي خليط من نوعين من المواد(برم2/3 وبرم2/5) باستخدام نموذج أيزنك

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الخلاصة

لقد تم في هذا البحث دراسة نظام فيري مغناطيسي مزيج من نوعين من المواد يختلفان في البرم باستخدام تقريب متوسط المجال لنموذج أيزنك. النظام المغناطيسي يتكون من مادتين مختلفتين في البرم الأولى 2/3 والثانية 2/5 ولهما تباين مغناطيسي مختلف (Anisotropy) ووضع مخطط الحالة الأرضية (الحالة الطورية) للنظام. لقد لوحظت ظاهرة التذبذب الفيري مغناطيسي للنظام (ferrimagnetic Reentrant) في المناطق الفعالة والتي تعتمد بقوة على التباين المغناطيسي للخليط.

Introduction

Several theoretical investigations have been reported concerning the extension of efforts to a more general mixed spin Ising model with one constituent having spin-1 and another having spin-3/2 . The mean-field approximation (MFA), in spite of its limitations, is an adequate starting point [1]. The theoretical work may be classified into two types. In the first type, the spin compensation temperature of the system can be obtained by requiring the total magnetization as being equal to zero for various values of anisotropies; though the reduced magnetization of the sublattices forming the system is not equal to zero [1, 2, 3, 4, 5].

In the second class of work, the first and second order phase transitions demand Landau expansion of the free energy in the order parameter [1, 5]. In this work we are concerned with the second type. It has been suggested that the resulting system behavior with the mixed spin-3/2 and spin-5/2 could be due to various values of the single-ion anisotropies.

Theory

We start by summarizing analytical results obtained for the mean field approximation (MFA).

The central idea of the mean-field theory is very simple:

We treat the nearest neighbour Ising model in zero fields on a lattice containing two sublattices A ,B having N sites, each site having Z nearest neighbours.

The Hamiltonian of the system in the Ising model, with $H_o=0$, can be written as [1]:

$$H = -J_{ij}\sum_{i,j} s_i^A s_j^B - D_A \sum_i (s_i^A)^2 - D_B \sum_j (s_j^B)^2 \qquad (1)$$

Where the sites of sublattices A are occupied by spins s_i^A taking the values of $\pm 1/2$, $\pm 3/2$, and the sites of sublattices B occupied by spins s_j^B taking the values of $\pm 1/2, \pm 3/2$, $\pm 5/2$. D_A, D_B are the anisotropies acting on the spin -3/2 and spin -5/2 respectively.

J_{ij} is the exchange interaction between spins at sites i and j .The expectation value of the spin variable at the sites i or j is given by:

$$\langle m_{i/j} \rangle = \frac{1}{z} Trs_{i/j} e^{-\beta H} \qquad (2)$$

With,

$$z = -Tre^{-\beta H} \qquad (3)$$

Where Tr means the sum over allowed states of the system .Here,

$$\beta = \frac{1}{K_B T} \quad .$$

Thus, substituting the Hamiltonian of the system in equation (2) ,one has:

$$m_A = \frac{1}{2} \frac{3\sinh(\frac{3}{2}k_1) + e^{-2\beta D_A}\sinh(\frac{1}{2}k_1)}{\cosh(\frac{3}{2}k_1) + e^{-2\beta D_A}\cosh(\frac{1}{2}k_1)} \qquad (4)$$

With $k_1 = \beta JZm_B$, where Z is the nearest-neighbour coordination number of the lattice,

$$m_B = \frac{1}{2} \frac{5\sinh(\frac{5}{2}k_2) + 3e^{-4\beta D_B}\sinh(\frac{3}{2}k_2) + e^{-6\beta D_B}\sinh(\frac{1}{2}k_2)}{\cosh(\frac{5}{2}k_2) + e^{-4\beta D_B}\cosh(\frac{3}{2}k_2) + e^{-6\beta D_B}\cosh(\frac{1}{2}k_2)} \qquad (5)$$

and $k_2 = \beta JZm_A$.

A systematic way of deriving the mean-field theory for a given microscopic Hamiltonian is to start from the Bogoliubov inequality [6]:

$$F \le \Phi = F_o + \langle H - H_o \rangle_o \qquad (6)$$

where F is the free energy of the system, H_o is a trial Hamiltonian depending on variational parameters, F_o is the corresponding free energy, and $\langle K \rangle_o$ denotes an average taken in the ensemble defined by H_o . The mean-field free energy is then defined by minimizing Φ with respect to the variational parameters $\lambda_{A/B}$, such that:

$$F_{mf} = \min_{\lambda_{A/B}} \{\Phi\} \qquad (7)$$

This gives the best possible approximation to the true free energy for a given choice of H_o , since the inequality (eq.6) insists that the mean-field free energy cannot fall below the true free energy. In this work we consider one of the simplest possible choices of H_o [1] :

$$H_o = -\sum_i [\lambda_A s_i^A + D_A (s_i^A)^2] - \sum_j [\lambda_B s_j^B + D_B (s_j^B)^2] \qquad (8)$$

Where λ_A and λ_B are the two variational parameters related to the two different spins respectively. Then the approximated free energy can be obtained by minimizing the right hand side of equation (6) with respect to the variational parameters mentioned above. Thus, equation (6) can be expressed as:

$$f \equiv \frac{\Phi}{N} = -\frac{1}{2\beta}\{\ln[2e^{9/4\beta D_A}\cosh(\frac{3}{2}\beta\lambda_A) + 2e^{1/4\beta D_A}\cosh(\frac{1}{2}\beta\lambda_A)] + \ln[2e^{25/4\beta D_B}\cosh(\frac{5}{2}\beta\lambda_B) + 2e^{9/4\beta D_B}\cosh(\frac{3}{2}\beta\lambda_B) + 2e^{1/4\beta D_B}\cosh(\frac{1}{2}\beta\lambda_B)]\} + 1/2(-ZJm_A m_B + \lambda_A m_A + \lambda_B m_B) \qquad (9)$$

Where N is the total number of sites of lattice . Minimizing this expression with respect to λ_A and λ_B gives self-consistent expressions for the mean-field (eqs. (4),(5)):

$$\lambda_A = ZJm_B \quad , \lambda_B = ZJm_A \qquad (10)$$

.

With,

$$m_A \equiv \left\langle s_i^A \right\rangle_o = \frac{1}{2}\frac{3\sinh(\frac{3}{2}\beta\lambda_A) + e^{-2\beta D_A}\sinh(\frac{1}{2}\beta\lambda_A)}{\cosh(\frac{3}{2}\beta\lambda_A) + e^{-2\beta D_A}\cosh(\frac{1}{2}\beta\lambda_A)} \quad (11)$$

$$m_B \equiv \left\langle s_j^B \right\rangle_o = \frac{1}{2}\frac{5\sinh(\frac{5}{2}\beta\lambda_B) + 3e^{-4\beta D_B}\sinh(\frac{3}{2}\beta\lambda_B) + e^{-6\beta D_B}\sinh(\frac{1}{2}\beta\lambda_B)}{\cosh(\frac{5}{2}\beta\lambda_B) + e^{-4\beta D_B}\cosh(\frac{3}{2}\beta\lambda_B) + e^{-6\beta D_B}\cosh(\frac{1}{2}\beta\lambda_B)} \quad (12)$$

Since the present model is related to the spin-3/2 and spin-5/2 Ising systems for any value of parameters, it undergoes a second-order transition and some features of the phase diagram may be obtained analytically. To determine the second-order transition lines, we need to expand eqs.((9),(11),(12)),thus :

$$f = f_o + \frac{1}{2!}am_A^2 + \frac{1}{4!}bm_A^4 + ... \quad (13)$$

Where the coefficients f_o and a are given by:

$$f_o = -\frac{1}{2\beta}\ln[(x_a + y_a)(x_b + y_b + z_b)] \quad (14)$$

$$a = -\frac{1}{2\beta}[t^2 b_1 + 0.25t^4 a_1 b_1^2] + 0.5tZJb_1 \quad (15)$$

and,

$$x_a = 2e^{9/4\beta D_A}, \qquad y_a = 2e^{1/4\beta D_A},$$

$$t = 0.5\beta ZJ, \qquad x_b = 2e^{25/4\beta D_B},$$

$$y_b = 2e^{9/4\beta D_B}, \qquad z_b = 2e^{1/4\beta D_B},$$

$$b_1 = \frac{25x_b + 9y_b + z_b}{x_b + y_b + z_b}, a_1 = \frac{9x_a + y_a}{x_a + y_a}$$

The second-order phase transition line is then determined by a=0 and b>0. It is worth mentioning that eq. (15) could be evaluated for both the ferromagnetic phase stability limit (J>0) and the ferromagnetic one (J<0) [1, 7].

Results and Discussion

We first consider the ground-state of the system which can easily be determined from Hamiltonian (1) by comparing the energies of the corresponding configurations as shown in Fig. (1).

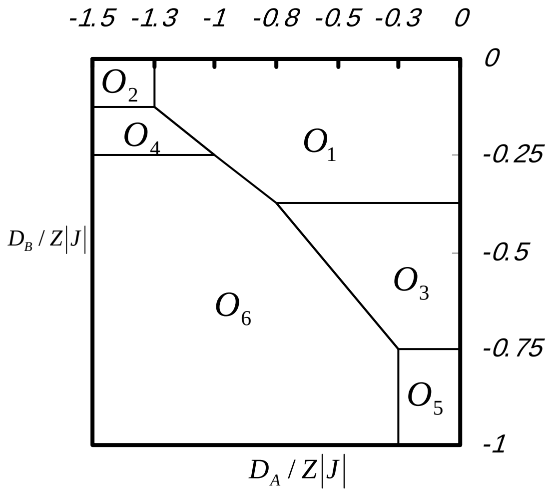

Figure 1: Ground state phase diagram of the mixed spin-3/2 and spin-5/2 Ising ferrimagnetic system with the coordination number *Z* and different single-ion anisotropies D_A and D_B . The six ordered phases: O_1,O_2,O_3,O_4,O_5, and O_6 are separated by thin lines .

It is worth noting that, at zero temperature, one can find six phases with different values of $\{ m_A, m_B, K_A, K_B \}$, namely , the ferrimagnetic phases ordered as:

$$O_1 \equiv \{\frac{3}{2},\frac{5}{2},\frac{9}{4},\frac{25}{4}\}, O_2 \equiv \{\frac{1}{2},\frac{5}{2},\frac{1}{4},\frac{25}{4}\},$$

$$O_3 \equiv \{\frac{3}{2},\frac{3}{2},\frac{9}{4},\frac{9}{4}\}, O_4 \equiv \{\frac{1}{2},\frac{5}{2},\frac{1}{4},\frac{25}{4}\},$$

$$O_5 \equiv \{\frac{3}{2},\frac{1}{2},\frac{9}{4},\frac{1}{4}\}, O_6 \equiv \{\frac{3}{2},\frac{1}{2},\frac{9}{4},\frac{1}{4}\}.$$

There are no disordered phases where the parameters K_A and K_B are defined by:

$$K_A = \left\langle (s_i^A)^2 \right\rangle, K_B = \left\langle (s_j^B)^2 \right\rangle \quad (16)$$

Let us consider the case when $4 \le D_B / Z|J| \le -2.5$ .Fig.(2) shows the phase diagrams in the (D_A, T) plane for various values of $D_B / Z|J|$. We see that a certain type of phase diagram is achieved with second-order transitions at different values of transition temperature ; that is to say , phase transitions related to anisotropy continuity showing second-order behavior.

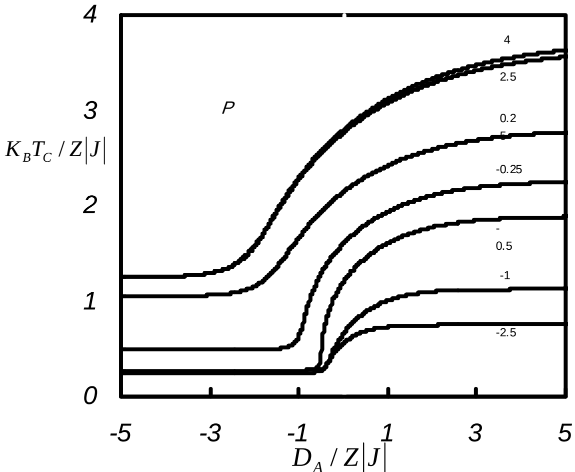

Figure 2: Phase diagram in the (D_A, T) plane for the mixed-spin Ising ferrimagnetic system with the coordination number Z , when the value of D_B is changed . The solid lines indicate second-order phase transitions. P is the paramagnetic phase.

Our results could be compared with those of spin-1/2 and spin-3/2 systems using the effective field theory [8]. Furthermore, one can see that for the values of $D_B / Z|J| \geq 4$, the transition temperature can never be increased ; and for $D_B / Z|J| \leq -2.5$, the transition temperature can never be lowered. Figure (3) shows the low-temperature phase diagram in the (D_B, T) plane for the mixed-spin Ising ferrimagnetic system with the coordination number Z using various values of $D_A / Z|J|$.

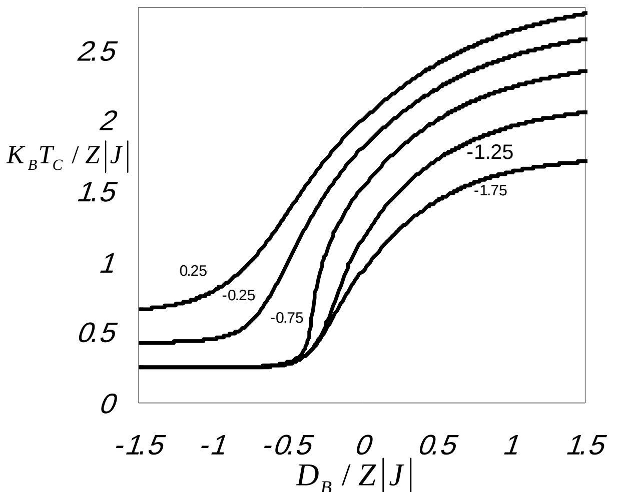

Figure 3: Phase diagram in the (D_B,T) plane for the mixed-spin Ising ferrimagnet with the coordination number Z , when the value of D_A is changed. The solid lines indicate second-order phase transitions. P is the paramagnetic phase.

Taking a small region from the phase diagram under consideration one can observe a behaviour of jump. It is seen from Fig.(4) that within the region joining the values of $D_B / Z|J| = -0.7$ and $D_B / Z|J| = -0.875$ certain curves of jump are clearly shown. This is indicated in Fig.(4). Typical sublattice magnetization curves referring to the phase diagram given in Fig.(4) are shown in Figure (5) , for $D_A / Z|J| = -0.7$. The curves labeled –0.3475 in Figure (5) correspond to the values of $D_B / Z|J|$ where a jump behavior occurs. The sublattice magnetization curves labeled –0.35025,–0.345 are for the value of $D_B / Z|J|$ corresponding to the isolated critical points.

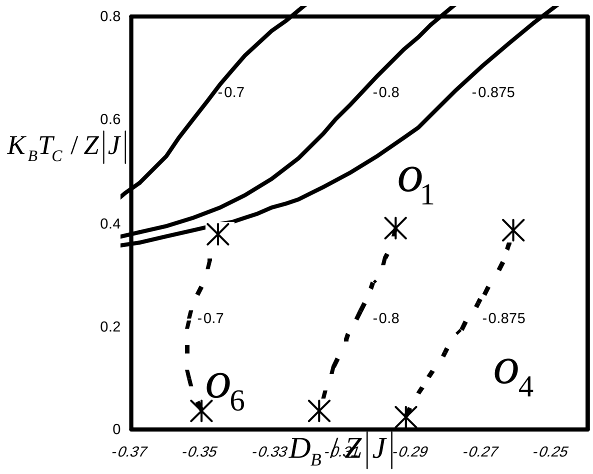

Figure 4: Phase diagrams in the (D_B,T) plane for the mixed- spin Ising ferrimagnetic with the coordination number Z , when the value of D_A is changed. The solid lines indicate second-order transitions, while the heavy dashed line represents the jumps in magnetization . The stars correspond to the isolated points .O_1, O_4,and O_6 are distinct ordered ferrimagnetic phases ,and P is the paramagnetic phase .

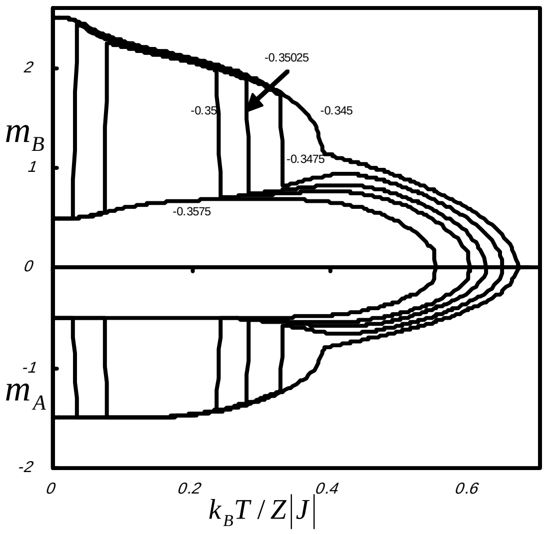

Figure 5: Thermal variations of the sublattice magnetization m_A ,m_B for the mixed –spin Ising ferrimagnet with the coordination number Z ,when the value of $D_B / Z|J|$ is changed , for fixed $D_A / Z|J| = -0.7$. The curves with values of $D_B / Z|J| = -0.345, -0.3475$ indicate the jump and reentrant behaviors respectively at low temperature.

Figure (6) shows the sublattice magnetization curves at low temperatures for anisotropy $D_B / Z|J|$ corresponding to the reentrant behavior given in Figure (4). It is also interesting to indicate that the mixed-spin system exhibits a reentrant behavior at low temperature.

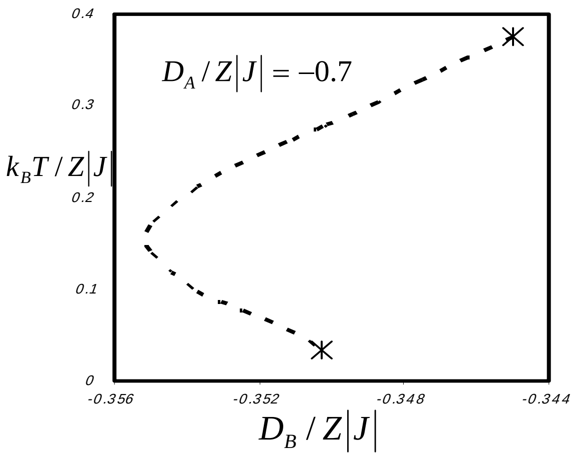

Figure 6: A close view low- temperature phase diagram in the (D_B , T) plane for the mixed-spin Ising Ferrimagnet with the coordination number Z , in the region of D_B at $D_A / Z|J| = -0.7$, indicates the reentrant behavior.

Now we may discuss the scale of Fig.(3)which is too small to see. However, this can be shown in Figure (4). In Figure (4) the critical line for $D_A = -0.7$ shows reentrant behavior in the phase diagram, i.e., two phase transitions [3], within the range $-0.35 < D_B \leq -0.3505$.It is possible within this system, as we noticed, to have many critical temperatures for a fixed value of D_B. Furthermore, the system considered here doesn't exhibit compensation phenomena since the behavior of the curves in Figure (2) indicate second-order phase transition only . Now, let us discuss the temperature dependence of the sublattice magnetizations m_A and m_B by solving the coupled eqs.(10)-(12) numerically. As shown in Fig.(7) , when $D_B / Z|J| \geq -1$ for fixed $D_A = -0.125$, the sublattice magnetizations of mixture show normal thermal variation behaviour [8]. Fig.(8) refers to the thermal variations of the sublattice magnetizations m_A, m_B for the same system with varying value of $D_B / Z|J|$ for fixed $D_A / Z|J| = -1.5$.

For $-0.075 \leq D_B \leq -0.375$ the temperature dependence of may exhibit a rather rapid decrease from its saturation value at $T = 0K^o$. The phenomenon is further enhanced when the value of D_B approaches the critical value .At the critical value of D_B ,in particular and for $T = 0K^o$, the saturation value of m is 0.5 indicating that in the ground state the spin configuration of the system consists of the mixed phases $s_i^A = \pm\frac{3}{2}$ and $s_j^B = \pm\frac{5}{2}$ with equal probability.

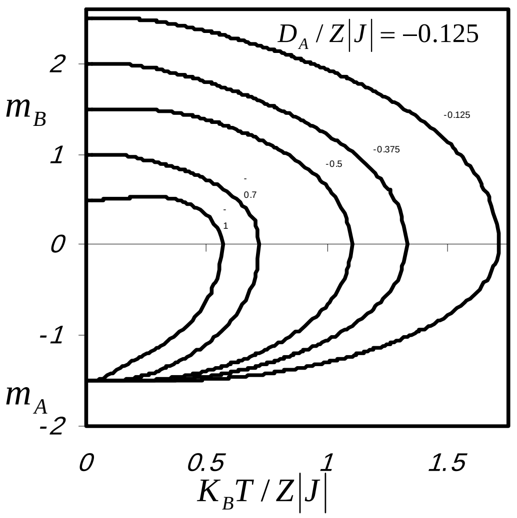

Figure 7: The temperature dependences of the sublattice magnetizations m_A ,m_B for the mixed – spin Ising ferrimagnetic with the coordination number Z ,when the value of $D_B / Z|J|$ is changed , for fixed $D_A / Z|J| = -0.125$.

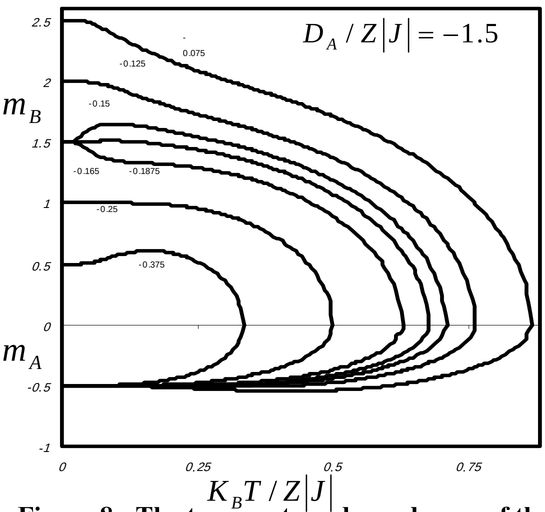

Figure 8: The temperature dependences of the sublattice magnetizations m_A ,m_B for the mixed – spin Ising ferrimagnet with the coordination number Z ,when the value of $D_B / Z|J|$ is changed , for fixed $D_A / Z|J| = -1.5$.

Conclusions

We have determined the global phase diagram of the mixed spin – 3/2 and spin – 5/2 Ising ferrimagnetic system with different single – ion anisotropies acting on the spin – 3/2 and spin – 5/2 using the mean – field approximation. It is found that single-ion anisotropy has strong effect on the mixture. Therefore, the whole phase diagram ordered (magnetic material) comparison to the system (1, 3/2). This phase diagram exhibited two compensation points, in agreement with the system (1, 3/2). This outstanding result has been discovered experimentally [9].

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