Mean field study of decorated ferrimagnetic Ising model

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The magnetic properties of a decorated ferrimagnetic Ising model consisting of two magnetic atoms A and B with spins $\sigma_A=\frac{1}{2}$ and $S_B=1$ are investigated by the use of the mean field approximation. Transition temperatures and the existence of the one or double compensation temperatures of the decorated ferrimagnetic square lattice are examined.

Keywords: Decorated Ising model; ferrimagnetism; compensation temperature.

1– Introduction:

Over several years, some attention has been directed to the ferrimagnetic materials due to their potential technological applications [1]. Experimentally, important advances have been made in the synthesis of 2 and 3-dimensional ferrimagnets, such as 2d organometallic ferrimagnets[2], 2d networks of the mixed-metal material $\{[P(Phenyl)_4][MnCr(oxalate)_3]\}_n$[3] and others[4-6]. Theoretically, the magnetic properties of these systems have been extensively studied by a variety of techniques, as, for example, mean field approximation [7], effective field theory[8,9], finite cluster approximation [10], renormalization group [11,12] and Monte-Carlo simulation[13,14].

An interesting phenomenon has been formed in the ferrimagnetic systems is a compensation temperature T_{cmp} below the critical temperature T_c [15]. This property is very useful in thermomagnetic recording. The existence of this temperature T_{cmp} is due, under certain conditions, to sublattice magnetizations which compensate each other. Then the resultant magnetization vanishes at this temperature.

The existence of compensation temperature has been found in an other systems normally decorated Ising systems. These systems were originally introduced in literature by Syozi[16]. Recently, a decorated two sublalttices ferrimagnetic Ising model consisting of two magnetic atoms A and B with spins $\sigma_A=\frac{1}{2}$ and $S_B>\frac{1}{2}$ has been introduced by Kaneyoshi[17]. The author has used the effective field theory with correlation (EFT) and has showed that the model can exhibit compensation points. Other authors have studied these systems by the use of the EFT [18], numerical solution [19], or exact solution [20].

In this paper, we investigate the decorated ferrimagnetic Ising model, in which the two magnetic atoms A and B have spins $\sigma_A=\frac{1}{2}$ and $S_B=1$, respectively, using the mean field approximation (MFA). We investigate some interesting phenomena not discussed with previous works, such as first order transition and double compensation temperature. We have obtained both phase diagrams and magnetic properties. The paper is organized as follows: In section 2, we introduce the model and give the details of the MFA. In section 3, we present and discuss our results, and finally in section 4 we summarize our conclusions.

2 - Model and mean field approximation:

The MFA represents the infinite dimensional limit of statistical systems since its neglects correlations between different spins. However it is interesting to study the mean field behaviour of the decorated ferrimagnetic Ising system. The whole lattice is divided into two sublattices L_1 and L_2. Every point of L_1 is always occupied by an A atom with the fixed spin $\sigma_A=\frac{1}{2}$ that of L_2, which is composed of one decorating point on every bond of L1, is always occupied by a B atom with a fixed spin $S_B = 1$.

The exchange interaction between A and B atoms is assumed to be antiferromagnetic. Furthermore, we assume that there exists a ferromagnetic exchange interaction between every nearest neighbours pair of A atoms. The two dimensional system is depicted in fig.1.

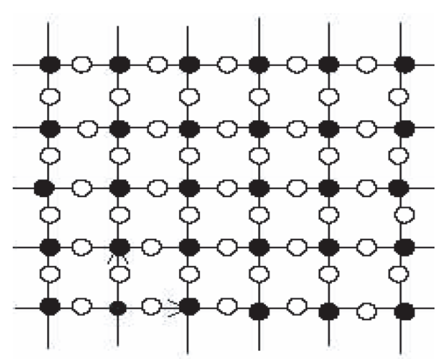


Figure 1: The two dimensional decorated Ising spin system consisting of two kinds of magnetic atoms A and B with spins values $\sigma_A=\frac{1}{2}$ (black points) and $S_B=1$(white points) respectively.

The system is described by the following Hamiltonian:

$$H = -J_1\sum_{<ij>}\sigma_i\sigma_j + J_2\sum_{<ij>}\sigma_i S_j - \Delta\sum_i S_i^2 \quad (1)$$

Where the spins $\sigma_i = \pm\frac{1}{2}$ and $S_i = \pm 1$, 0 are localized in sublalttices L_1 and L_2, respectively. $J_1(J_1>0)$ and $J_2(J_2>0)$ are the exchange interactions. Δ is the crystal field and the summations are carried out only over nearest - neighbours pairs of spins.
To write the mean field equation let h_σ and h_S denote the molecular fields associated with order parameters m_σ =<σ> and m_S =<S>, respectively:

and $h_S = 2J_2 m_\sigma$ (2)

The effective Hamiltonian of the system is:

$$H_0 = -\sum_{i}^{N} h_\sigma\sigma_i + \sum_{i=1}^{2N} h_S S_i - \Delta\sum_{i=1}^{2N} S_i^2 \quad (3)$$

It generate the following partition function:

$Z_0 =$

$$Z_0 = \prod_i^N\left(2\cosh\left(\frac{\beta h_\sigma}{2}\right)\right)\prod_i^{2N}\left(1+2\exp(\beta\Delta)\cosh(\beta h_S)\right) \quad (4)$$

Where $\beta = \frac{1}{k_\beta T}$ is the inverse temperature.

The variational principle for the free energy per site is described by:

$$F \le \overline{F} = - \quad (5)$$

And the order parameters which are the spin averages are given by:

(6)

$$m_S = \frac{-\sinh\left(\frac{2J_2 m_\sigma}{T}\right)\exp(\beta\Delta)}{0.5+\cosh\left(\frac{2J_2 m_\sigma}{T}\right)\exp(\beta\Delta)}$$

Then the total free energy can be written as:

$$F = -\frac{1}{\beta}\ln(Z_0) - J_1\sum_{<ij>}<\sigma_i><\sigma_j> + J_2\sum_{<ij>}<\sigma_i><S_j> + \sum_{i=1}^{N} h_\sigma<\sigma_i> - \sum_{i=1}^{2N} h_S<S_i>$$

(7)

Usually the solutions of Eqs (6) will not be unique, the stable ones are those which minimise the free energy (Eq(7)), while the others are the unstable ones. If the order parameters are continuous (discontinuous), the transition is of second (first) order.

Let us first discuss the ground-state phase diagram in the $(d=\frac{\Delta}{J_1}, r=\frac{J_2}{J_1})$ plane. We note that d is reduced crystal field. Thus, for $\frac{T}{J_1}=0$ and $r\ge 0$, equation (6) has two solutions: the phase

and ferrimagnetic phase. The energy of all possible solute

ions can easily be calculated. By comparing these energies, the type of the ground state is then determined as we see from figure 2. So, we have a first order transition line separating these two phases and given by r+d=0.

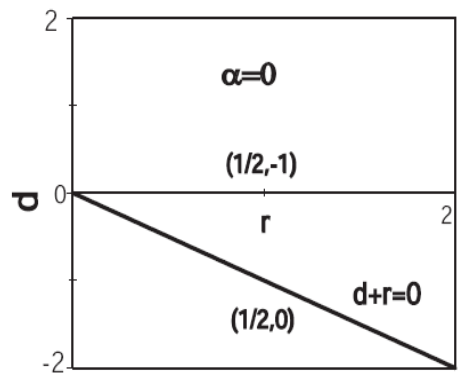


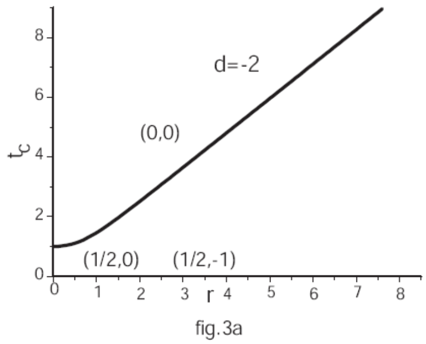
Figure 2: The ground state phase diagram. The full line represents the first-order phase transition

that separates, the phase from the ferrimagnetic phase.

3 - Results and discussions:

3-1 phase diagrams:

Let us examine the phase diagrams of the two dimensional decorated Ising model (fig1). For this, equations (6) and (7) are solved numerically. However, the phase diagram in $(t_c=\frac{T_C}{J_1}, r)$ and (t_c, d) are obtained from mean field approximation are shown in fig3 and fig4, respectively.



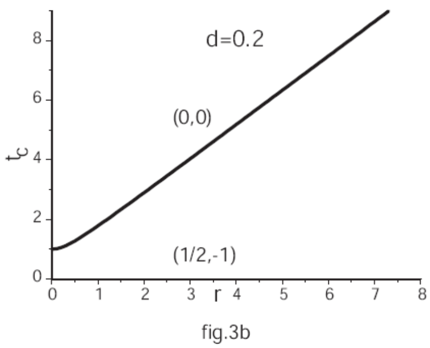


Figure 3: The phase diagram in the (t_c, r) space for the decorated ferrimagnetic system with z=4 when the value of d is selected at d=-2 in fig.3a or d=0.2 in fig.3b.

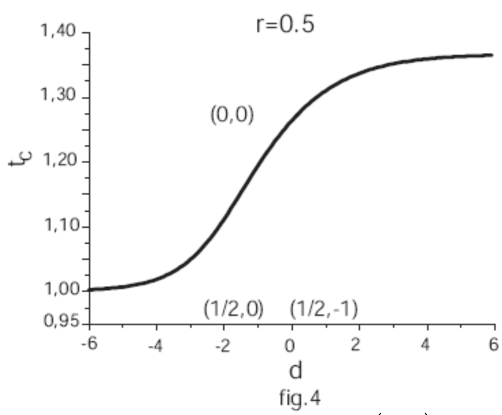


Figure 4: The phase diagram in the (t_c, d) plane for the decorated ferrimagnetic system with z=4 and r=0.5. The first order phase transition separating the two phases and start at d=-0.5 (d+r=0) at $\frac{T_C}{J_1}=0$ °K.

It consists of second order transition line, separating the paramagnetic phase $(m_\sigma=0, m_S=0)$ from the ferrimagnetic phase. In fact , for d<0 as is shown in fig.3a, the phase appears for the weak value of r, where

as the phase exist fo r great value of r. The transition line separating the latest phases is a first order transition line starting at r=-d at $\frac{T_C}{J_1}$=0°K and terminated at an end point. But, it is a short line and we have not drew it. However for d>0 (fig.3b), the

phase disappears and we have on

ly a second order transition line between the paramagnetic $(m_\sigma=0, m_S=0)$ and

ferrimagnetic phases. In the both case (d>0 and d<0), for great values of r the behaviour of the second line transition is linear.

Figure.4 shows reduced crystal field interaction d dependence of reduced temperature $\frac{T_C}{J_1}$. As in shown in fig.3a, we can distinguish the second order phase transition line separating the phase

$(m_\sigma=0, m_S=0)$ from the phases

and . Furthermore, these last phases subsist for any va

lue of r>0 and we have a first order transition line between them. This line starts at d=-r at T=0°K. Also, the second order transition temperature between the paramagnetic phase $(m_\sigma=0, m_S=0)$ and the

ferrimagnetic phaseincreases with r.

In addition to critical temperature, compensation points appear in the system. The reduced compensation temperature $t_{cmp}=\frac{T_{cmp}}{J_1}$ is located below the reduced critical temperature t_c. t_{cmp} is determined from the condition M=0 for $t_{cmp}<t_c$, when M is the total magnetization of the system. So, M is given by:

$$m=\frac{M}{N_A}=m_\sigma+2m_s$$

Where m is the magnetization per site and N_A is the number of sites with lattice L_1 .

In figures 5a and 5b, we reported the lines of compensation points as a function of r and d, respectively.

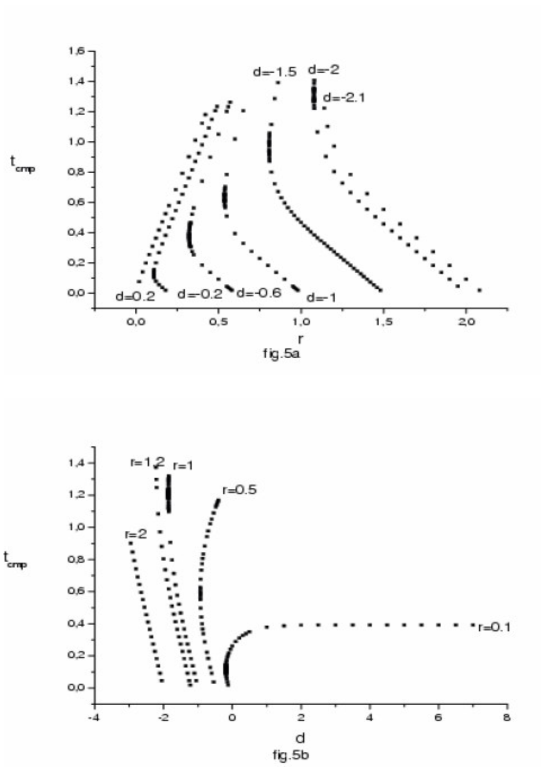


Figure 5: The compensation point line in the (t_{cmp}, r) and (t_{cmp}, d) planes, for the decorated ferrimagnetic system in square lattice, for selected values of d (fig.5a) and (fig.5b), respectively. In both cases we can show double compensation temperatures.

Thus, in fig.5a we can show not only one compensation point but two. In fact, the phenomenon of double compensation appear for the negative value of d, precisely for $-2.05 \leq d < 0$. This outstanding result which is beyond the Néel theory has been discovered experimentally in [21]. However, only one compensation point appear for positive values of d and for d $\leq$ -2.06.

urthermore, in this case, the behaviour of compensation line is linear.

In fig.5b, phase diagram (t_{cmp}, d) is depicted for some selected values of r. We can show that for $0 < r \leq 1.19$, the phase diagram exhibits the two successive compensation temperatures. This last phenomenon appears for negative values of d. Furthermore, for r $\geq$ 1.2, only one compensation point appears.

3-2 Magnetic properties

Now, let us examine the temperature dependencies of the magnetizations m_σ, m_s and total magnetization M in order to complete the phase diagrams represented in figs3 and 4. Thus, in figs.6a and 6b the magnetization m_σ , m_s and M are depicted for d=-2 and r=1.95 and r=2.05, respectively.

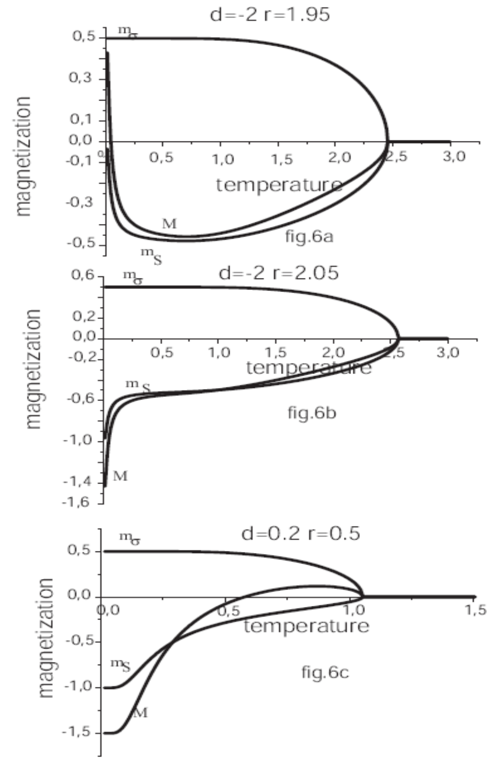


Figure 6: The temperature dependencies of the magnetization m_σ , m_s and M for decorated ferrimagnetic system in square lattice with d=-2 and selected value of r=1.95 (fig.6a) and r=2.05 (fig.6b). In both cases we have second order transition line that separates

the (fig.6a) or (fig.6b) from

the paramagnetic phase $(m_\sigma = 0, m_S = 0)$.

In both figures we show the second order transition temperatures

between the phases and $(m_\sigma = 0, m_S = 0)$ (fig.6a) and from the ferrimagnetic phase

to paramagnetic one $(m_\sigma = 0, m_S = 0)$ (fig.6b). We note that the first order transition line between the

phases and starts at r=2 at

T=0°K. These results are in concordance with fig.3a.

However, for positive value of d, the phase disappears and we have only

second order transition line between paramagnetic $(m_\sigma = 0, m_S = 0)$ and ferrimagnetic phases (fi g.6c). In fig.7a and 7b we draw the

magnetization m_σ , m_s versus d for r=0.5 and t_c=0.01 and 0.08, respectively.

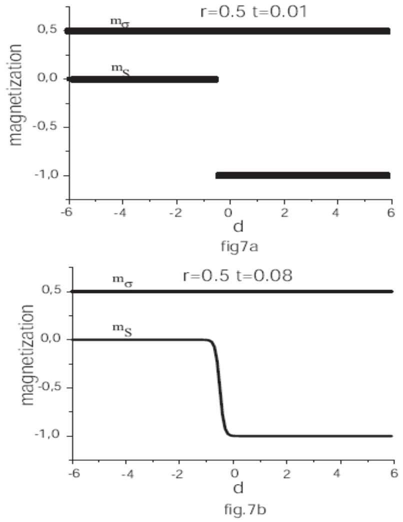


Figure 7: The reduced crystal field dependencies of the magnetization m_σ , m_s and M with r=0.5, t=0.01 (fig.7a) r=0.5, d=0.08 (fig.7b).

We can show a discontinuity of m_s from 0 to –1 at t=0.01 (fig.7a) whereas m_s is continue for t=0.08 (fig.7b). In fact, the first order transition line between the phases and is very short. In fig8a and 8b the magnetization m_σ , m_s and M are plotted as function of temperature for (r=0.15, d=0.2) and (r=0.5, d=-0.85) respectively.

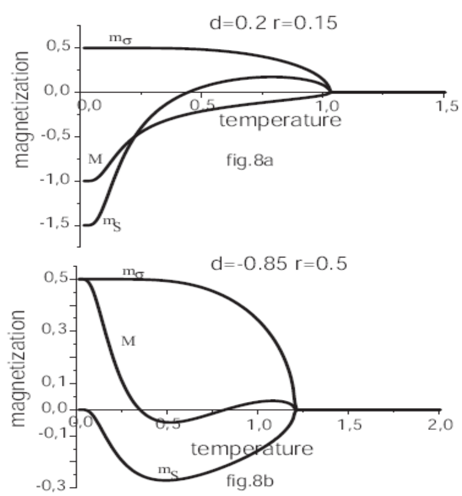


Figure 8: The temperature dependencies of the magnetization m_σ , m_s and M with r=0.15 and d=0.2 (fig.8a) and r=0.5 and d=-0.85 (fig.8b). In the first case the system exhibit a one compensation temperature whereas in the second case we have two successive compensation temperatures.

We can show a single compensation temperature at t_{cmp} below the Curie temperature, where the net moment changes and this has been technological significance. However, in fig.8b, the two compensation points are evident.

4 - Conclusion

In this work, we have studied the decorated ferrimagnetic Ising model, in which the two magnetic atoms A and B have spins $\sigma_A = \frac{1}{2}$ and S_B=1, respectively, by the use of MFA. Indeed, we have given phase diagrams in (t_c,r) and (t_c,d) planes in which, at very low temperature there exist a first order transition line se parating the two phases and whereas, for large value of temperature, one have a second order transition line. Furthermore, the phase disappears for positive values of d. Also the compensation phenomenon has been investigated. In fact, we have reported the lines of compensation points as a function of r and d. We can show the existence of one or two successive compensation points where the total magnetization M vanishes at temperature before t_c .

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