Dependence on dilution of critical and compensation temperatures of a two-dimensional mixed spin-1/2 and spin-1 system

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1. Introduction

Ferrimagnetic systems i.e., materials have got considerable attention due to their technological applications. These systems consist of different spin sublattices and therefore they are also called as mixed spin systems. One of the most important properties of these systems is that they have a compensation temperature. In a ferrimagnetic spin system, sublattices have inequivalent moments interacting antiferromagnetically. At low temperatures, even though inequivalent moments of sublattices are antiparallel, they may not cancel each other owing to different temperature dependencies of the sublattice magnetizations. Fortunately, sublattices of a ferrimagnetic system compensate each other completely at \( T = T_{\text{comp}} \) below the Néel temperature \([1]\). This critical point value is called as compensation temperature or compensation point of ferrimagnetic spin system. At the compensation point, the total magnetization of ferrimagnetic system vanishes and only a small driving field is required to reverse the sign of magnetization of a locally heated magnetic domain by using a focused laser beam. Hence, writing and erasing processes can be achieved at this point. This kind of ferrimagnetic systems are known as magneto-optic materials.

In technological applications, it is important to produce the material i.e., spin system which has a desired compensation temperature. In recent studies, it has been shown that dilution plays a role on the compensation point of a ferrimagnetic mixed spin system. Therefore, the effects of dilution on the compensation temperature of mixed spin systems have been studied and interesting phenomenon have been found. For example, Bobák and Jasčur \([2]\) and Xin et al. \([3–5]\) investigated the thermal and magnetic properties of a mixed spin-1/2 and spin-1 ferrimagnetic system on square and honeycomb lattices within the framework of an effective-field theory with correlations. They obtained a number of interesting phenomena, such as possibility of two compensation points in the total magnetization curve. They also discussed the influence of the crystal field interaction and concentration of the non-magnetic atoms on the magnetic and thermal properties of the system and observed the tricritical point, reentrant phenomena and two compensation points. Bobák and Jurčišin \([6]\) and Kaneyoshi et al. \([7]\) investigated a diluted Ising ferrimagnetic system by using an effective-field approximation and showed that the system exhibits two or three compensation points in certain concentration ranges of magnetic atoms and crystal field for spin-(1, 3/2) and spin-(2, 5/2) systems, respectively. Spin-1/2 and spin-1 ferrimagnetic model on a hexagonal lattice was studied by Godoy et al. \([8]\) by employing mean-field calculations and Monte Carlo simulations. They showed that the phase diagram in the plane magnitude of spin-1 exchange interactions versus crystal field intensity exhibits a
very narrow region of compensation points. In addition, the influence of a transverse field on the compensation point was examined on honeycomb and square lattices [9–11].

As it can be seen from previous studies dilution effects on the thermal and magnetic behavior of the ferrimagnetic mixed systems have been investigated in detail. However, dependence of the critical and compensation temperatures on dilution has never been taken into account up to now. Therefore, this point still deserves particular attention for mixed spin systems. In this paper, we discuss dependence of the critical and compensation temperatures on dilution in a two-dimensional mixed spin-1/2 and spin-1 system with Monte Carlo simulation method. We find that the critical and compensation temperatures linearly decrease as the number of diluted sites increases in two-dimensional mixed spin-1/2 and spin-1 system.

2. The model and simulation technique

In order to investigate the effect of dilution on the critical and compensation temperatures and on the other physical quantities, we consider antiferromagnetically interacting two-dimensional mixed spin (1/2, 1) system with Hamiltonian

\[ H = -J_x \sum_{\langle ij \rangle} \sigma_i \sigma_j - J_y \sum_{\langle ij \rangle} \sigma_i \sigma_k + D \sum_j S_j^2 \]  

where \( \sigma = \pm 1/2 \) and \( S = \pm 1, 0 \). The first sum in Eq. (1) is over the nearest-neighbor and the second one is over the next-nearest-neighbor spins. \( J_x, J_y \), and \( D \) parameters define exchange interactions between the neighbor spins, and \( D \) is the crystal field.

To simulate the system, we initially chose spins \( S \) and \( \sigma \) randomly, but with equal number, in a discrete lattice according to Eq. (1). We also set equal number of non-magnetic atoms randomly in each sublattice. Then, we employed Metropolis Monte Carlo simulation algorithm [12] to Eq. (1) on a \( L \times L \) square lattice with periodic boundary conditions. Configurations were generated by selecting the sites in sequence through the lattice and making single-spin-flip attempts, which were accepted or rejected according to the Metropolis algorithm. Data were generated over 100 realization for \( L = 16, 32 \) and 64 with different numbers of non-magnetic atoms by using 25 000 Monte Carlo steps per site after discarding the first 2500 steps. Our program calculates the sublattice magnetizations \( M_A \) and \( M_B \), the total magnetization \( M \), the magnetic susceptibility \( \chi \) and the specific heat \( C \) for different densities of diluted sites. These quantities are defined as

\[ M_A = \frac{2}{L^2} \left( \sum_j S_j \right) \]  
(2)

\[ M_B = \frac{2}{L^2} \left( \sum_i \sigma_i \right) \]  
(3)

\[ M = \frac{1}{2}(M_A + M_B) \]  
(4)

\[ \chi = \frac{1}{kT} (\langle M^2 \rangle - \langle M \rangle^2) \]  
(5)

\[ C = \frac{1}{kT} (\langle E^2 \rangle - \langle E \rangle^2) \]  
(6)

where \( T \) denotes temperature, \( E \) is the internal energy of the system, and \( k \) is Boltzmann constant (here \( k = 1 \)).

To determine the compensation temperature \( T_{comp} \) from the computed magnetization data, the intersection point of the absolute values of the sublattice magnetizations was found using the relations

\[ |M_A(T_{comp})| = |M_B(T_{comp})| \]  
(7)

\[ \text{sign}(M_A(T_{comp})) = -\text{sign}(M_B(T_{comp})) \]  
(8)

with \( T_{comp} < T_c \), where \( T_c \) is the critical temperature i.e., Neél temperature. Eqs. (7) and (8) indicate that the sign of the sublattice magnetizations is different, however, absolute values of them are equal to each other at the compensation point.

3. Numerical results and discussion

In order to see the effect of the non-magnetic atoms on the magnetic and thermal behaviors of a two-dimensional mixed spin system defined with Eq. (1), choosing \( J_x = -2, J_y = 8 \) and \( D = 2.6 \) we give the results of 64 \( \times \) 64 square lattice for \( N = 0, 64, 256, 512 \) in Figs. 1–6. Here we must state that the nearest-neighbor interaction \( J_x \) in Eq. (1) does not play a role on the compensation temperature, whereas observation of the compensation temperature depends on the parameters \( J_x \) and \( D \). This point has been discussed in Refs. [13,14]. Therefore, in this study, we have particularly focused on the effect of the different dilution rates with non-magnetic atoms \( N \) for arbitrary fixed \( J_x, J_y \) and \( D \). On the other hand, to analyze the effect of the non-magnetic atoms on the critical and compensation temperatures, for fixed \( J_x = -2, J_y = 8 \) and two different crystal field values \( D = 1.6 \) and 2.6 we give the results of different lattice sizes \( (L = 16, 32, 64) \) for different densities of diluted sites in Figs. 7 and 8.

Fig. 1. The temperature dependencies of sublattice magnetizations \( M_A, M_B \) and susceptibility \( \chi \) of non-diluted square lattice for \( J_x = -2, J_y = 8 \) and \( D = 2.6 \).
the second zero denotes the temperature value at which $M$ is zero which corresponds to critical temperature point. One can see some quantitative differences in the total magnetization curves for different number of non-magnetic atoms, but it is hard to comment on this naive picture about dependence on dilution of the critical and compensation temperatures. However, it might be also predicted that the compensation and critical points appear near $T/J_1 = 3.6$ and $T/J_1 = 5.3$ for different numbers non-magnetic atoms.

In Figs. 3 and 4, for different $N$ values ($N = 0, 64, 256, 512$) and fixed $J_1 = -2, J_4 = 8$ and $D = 2.6$, values, the behavior of spin-1 and spin-1/2 sublattice magnetizations $M_A$ and $M_B$ have been demonstrated separately. As seen from these figures, sublattice magnetizations take values which are different from zero at the compensation point, while as seen in Fig. 2, the total magnetization value is zero at the compensation point for all values of $N$. These two figures inform us about behavior of the compensation points for different $N$ values. Indeed, it is possible to obtain the compensation points for different $N$ values if $M_A$ is mapped onto $M_B$ in the same figure as well as in Fig. 1. The first crosses in the sublattice magnetization curves of $M_A$ and $M_B$ correspond to the compensation points. One can easily predict from these figures that the compensation temperatures decrease as the number of non-magnetic atoms $N$ increases. The dilution dependence of compensation temperature which we have obtained from Figs. 3 and 4 is given above. However, it is still hard to comment on these figures about the dependence on dilution of the critical temperature points. But it is possible to see the behavior of the critical temperature points for different $N$ values in Fig. 5 in which the magnetic susceptibility has been plotted as a function of temperature for the same values of parameters. As it can be seen from Fig. 5 that there are two relatively sharp peaks and humps in magnetic susceptibility curves for different $N$ values. For the chosen parameters, the critical temperature points can be easily determined from the second peaks and humps. The second peaks and humps in the susceptibility curves appear at critical temperatures and indicate a phase transition from ferrimagnetic to paramagnetic, as expected. It can be clearly seen that the...
maximum points of the susceptibility curves become smaller and slide to left when the values of \( N \) increase, which means that the critical temperature decreases and magnetization gets weaker with increasing \( N \). The dilution dependence of the critical temperature which we have obtained from Fig. 5 is given above. On the other hand, the first humps in Fig. 5 may probably originate from the crystal field \( D \), and they do not indicate a compensation temperature or a phase transition in the model. The existence of the non-magnetic atoms on the lattice also affects the shapes of these humps in the susceptibility curves.

In Fig. 6, temperature dependence of the specific heat \( C \) has been plotted for different \( N \) and fixed \( J_1 = -2, J_4 = 8, D = 2.6 \) values. Similarly, there are also two relatively sharp humps and peak in specific heat. The first humps probably may also originate from \( D \), as well as the first humps in magnetic susceptibility. The second humps and peaks denote a phase transition. As seen from Fig. 6, maxima of the specific heat curves become smaller and slide to left when the value of \( N \) increases. It confirms that the critical temperature decreases with increasing \( N \).

Fig. 7 shows the dependence on density of diluted sites of the critical temperature for fixed \( J_1 = -2, J_4 = 8 \) and for two different crystal field values \( D = 1.6 \) and 2.6. As it can be seen from figure, non-magnetic atoms play an important role on the critical temperature of the system. Indeed, critical temperature of diluted system linearly decreases for fixed \( J \) and \( D \) with increasing density of diluted site in the lattice. Similarly, the crystal field also affects the critical temperature of the system. It can be seen from Fig. 7 that the critical temperature of the system decreases systematically when the crystal field value is increased. On the other hand, we can say that the critical temperature of the diluted mixed system does not affected from the lattice size.

Fig. 8 shows the dependence on density of diluted sites of the compensation temperature for fixed \( J_1 = -2, J_4 = 8 \) and for two different crystal field values \( D = 1.6 \) and 2.6 with different lattice sizes. Similarly, non-magnetic atoms and the crystal field play a significant role on the compensation temperature of the system as well as the critical temperature. As it can be seen from Fig. 8, the compensation temperature of diluted system linearly decreases for fixed \( J \) and \( D \) with increasing density of diluted sites in the lattice, and on the other hand, compensation temperature of the system decreases systematically when the crystal field value is increased. Finally, we can say that compensation temperature of the diluted mixed system does not affected from lattice size as well as the critical temperature.

4. Conclusion

In the present work, we have focused on the effect of non-magnetic atoms on the critical and compensation temperatures of a two-dimensional mixed spin-1/2 and spin-1 system. Employing Monte Carlo simulation method to the system, we have studied thermal and magnetic behaviors of the system and dependence of these properties with the concentration of non-magnetic atoms. We found that the thermal and magnetic behaviors clearly depend on the number of non-magnetic atoms in the lattice as seen from the figures given. Particularly, we have shown that the critical and compensation temperatures linearly decrease with increasing numbers of non-magnetic atoms of the two-dimensional mixed spin-1/2 and spin-1 system. The results show that dilution plays a significant role on the critical and compensation points of a two-dimensional mixed spin-1/2 and spin-1 system. On the other hand, these numerical results indicate that the compensation temperature of the real ferrimagnetic spin systems can be
changed by diluting the lattice with non-magnetic atoms, in order to obtain desired compensation temperature.

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