Role of anisotropy to the compensation in the Blume-Capel trilayered ferrimagnet

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Abstract: The trilayered Blume-Capel ($S = 1$) magnet with nearest neighbour intralayer ferromagnetic and nearest neighbour interlayer antiferromagnetic interaction is studied by Monte Carlo simulation. Depending on the relative interaction strength and the value of anisotropy the critical temperature (where all the sublattice magnetisations and consequently the total magnetisation vanishes) and the compensation temperature (where the total magnetisation vanishes for a special combination of nonzero sublattice magnetisations) are estimated. The comprehensive phase diagrams with lines of critical temperatures and compensation temperatures for different parameter values are drawn.

Keywords: Blume-Capel model, Monte Carlo simulation, Critical temperature, Compensation temperature
I. Introduction:

To study the magnetocaloric effects\cite{1}, magneto-optical recording \cite{2} and the giant magnetoresistance\cite{3}, the ferrimagnetic materials are widely used for experimental and theoretical studies. The thermomagnetic recording \cite{1} device requires the strong temperature dependence of the coercive field. Some ferrimagnetic materials shows compensation (the total magnetisation vanishes for nonzero sublattice magnetisations) at room temperatures where the coercive field is strongly dependent of temperature. The trilayered ferrimagnetic materials show an interesting phenomenon, called compensation. Below the critical temperature (where each of all sublattice magnetisations as well as the total magnetisation vanishes), for particular combinations of ferromagnetic and antiferromagnetic interaction strengths, the total magnetisation vanishes even for nonzero values of sublattice magnetisation. It has been reported that near the compensation the system shows diverging coercivity, and a good choice for thermomagnetic and magneto-optic recording\cite{4}. Due to this modern technological importance the study of compensation phenomena became quite interesting to the experimental and theoretical researchers. With the practical realisation of the layered magnetic materials, such as bilayer\cite{5}, trilayer\cite{6, 7} and multilayer\cite{8, 9, 10, 11}, theoretical inversions are required for better understanding.

Since, the exact theoretical treatments are not adequately available in the literature, the approximation methods are applied to study such complex compensation phenomena. The trilayer spin-$\frac{1}{2}$ ferrimagnets are the prototypes to study\cite{12} such effects. The Monte Carlo approach was employed\cite{13} to study the compensation in Ising trilayered magnetic models. The effects of dilution in Ising trilayered system was studied\cite{14, 15} by Monte Carlo (MC) simulation. The disordered system like spin-$\frac{1}{2}$ and spin-1 diluted layered magnets were also studied by meanfield\cite{16} and MC\cite{17} method. Recently, the effects of dilution in nanotri-layer graphene structure was studied by MC simulation\cite{18}. The double compensation temperatures are found\cite{19} in a mixed spin ($\frac{1}{2}, 1$) antiferromagnetic ovalene nanostructured system studied by MC simulation. The Monte Carlo methods were employed to study the Blume-Capel bilayered graphene structure with RKKY interactions. It was observed\cite{20} that the transition temperature increases with decreasing the number of nonmagnetic layers. However, the behaviours of Blume-Capel trilayer is not studied by MC method.

Although the Blume-Capel (BC) model\cite{21, 22, 23} was originally introduced to analyse the thermodynamic behaviours of $\lambda$-transition in the mixture of He$^3$-He$^4$, it is widely used to study the birectical/trirectical behaviours in various phase transitions. The nature (discontinuous/continuous) of the phase transition and the existence of trirectical point in face centered cubic BC model was studied\cite{24} by high temperature series extrapolation techniques. The critical behaviour\cite{27} and the trirectical behaviour\cite{26} in the BC model was studied by Monte Carlo simulation. It should be mentioned here that the variety of positional and/or orientational order and a very rich phase diagram was obtained\cite{28} recently even in $S = \frac{1}{2}$ Ising system in three dimensions by renormalization group theory in Migdal-Kadanoff approximation. The meanfield approximation was employed to study\cite{29} the general spin BC model. The meanfield solution was obtained\cite{30} in BC model with random crystal field also. The method of effective field theory was used\cite{31} to study the effects of random crystal field in the BC model. The wetting transition in BC model was studied\cite{32} by MC simulation.

The BC model exhibits the competing metastability. It should be mentioned here that
dynamic Monte Carlo and numerical transfer matrix method [33] were employed to study the competing metastability in the BC model. The behaviours of the competing metastable states at infinite volume are studied [34] in dynamic BC model. The metastable and unstable states are obtained [35] by cluster variation and path probability method. However, no study was found to consider the compensation in the BC trilayerd magnetic model systems.

What kind of behaviours are expected in the Blume-Capel trilayerd ferrimagnet? How does the anisotropy affect the compensation temperature? To address these question, in this article, the equilibrium behaviours of critical and compensation behaviours and the dependence of these two temperature on the anisotropy, are studied by Monte Carlo simulation. The paper is organized as follows: the model is described in the section II, the numerical results are reported in section III and the paper ends with summary in section IV.

II. Model and simulation:

A system of trilayer (say, top (or layer $l_1$), middle (or layer $l_2$) and bottom (or layer $l_3$)) is considered (see Fig. 1). Each layer is a square lattice of size $L \times L$. A spin ($S = 1$) is placed in each lattice site. The z-component of the spin ($S_z$), at $i$-th lattice site, can have any of the three values, i.e., $S_z = +1$, 0 and -1. The periodic boundary conditions are applied in both the directions of any layer. However, the top and bottom layers are placed in open boundary conditions. The intralayer interactions in the top and in the bottom layers are same. All interactions are considered to act over the nearest neighbours only. The energy of such a Blume-Capel ($S = 1$) trilayer is represented by the following Hamiltonian,

$$H = -J_{aa} \sum_{<ij>} S_z^i S_z^j - J_{bb} \sum_{<ij>} S_z^i S_z^j - J_{ab} \sum_{<ij>} S_z^i S_z^j + D \sum_i (S_z^i)^2$$  \hspace{0.5cm} (1)$$

where, $S_z^i$ represents the z-component of the Spin ($S = 1$) at any position ($i$-th lattice site). The values of $S_z^i$ may be any one of -1, 0 and +1. The first term represents the contribution to the energy due to nearest neighbour ferromagnetic ($J_{aa} > 0$) interactions among the spins in top layer and the same in the bottom layer. The second term represents the contribution to the energy due to the nearest neighbour interactions among the spins in the middle layer. $J_{bb} > 0$ is the ferromagnetic nearest neighbour interaction between the spins in the middle layer. The contribution to the energy due to nearest neighbour inter-layer antiferromagnetic ($J_{ab} < 0$) interaction is represented by the third term. The summations in all these three terms are considered only over distinct pairs to avoid any overcounting. Finally, the fourth term is the contribution to the energy due to the single site anisotropy, where $D$ is the strength of anisotropy.

In the simulation, a trilayered system of $L = 100$ is considered. The equilibrium configuration at any particular temperature ($T$) was achieved just by cooling the system slowly (with small change in temperature $\Delta T$) from a high temperature disordered state of random spin configurations. The high temperature random initial spin configuration was generated in such a way that the system contains almost equal numbers of $S_z^i = +1, 0$ and -1, distributed randomly. In such a configuration, all the sublattice magnetisations (for each of the three layers) as well as the total magnetisation of the whole system vanishes. Now a high value of the temperature is considered. A site has been chosen randomly. The energy ($E_i$) has been calculated for this initial configuration. A test value of the spin component
of the chosen site is considered from a random choice of the three values (+1, 0, -1). Now
the energy \( (E_f) \) with this test value is calculated. The \( \Delta E = E_f - E_i \), the change in energy
for accepting this test value is calculated. The probability of accepting this test value of the
spin is given by the Metropolis formula\[36\]
\[
P(S_i^z(\text{initial}) \rightarrow S_i^z(\text{test})) = \text{Min}[1, \exp(-\frac{\Delta E}{kT})] \tag{2}
\]
where \( k \) is the Boltzmann constant. The value of the test spin is accepted only if the prob-
ability is greater than or equal to a random number uniformly distributed between 0 and
1. In such way, \( 3L^2 \) such random updates of the spins are done and considered as the
unit of time (MCSS, Monte Carlo Step per Spin) in the simulation. In the present simul-
ational study, \( 12 \times 10^5 \) MCSS are considered, where the initial (transient) \( 6 \times 10^5 \) MCSS
were discarded and the quantities are calculated by averaging over next \( 6 \times 10^5 \) MCSS.
Some results are checked with smaller length of simulation and no significant changes were
observed. In that spirit, it was assumed that the system has reached the equilibrium config-
uration of that given temperature \( (T) \). Now a lower temperature \( (\Delta T = 0.05) \) is considered
and the present spin configuration was used as the initial starting configuration for that
lower temperature. In this way, the macroscopic quantities are calculated for different tem-
peratures. Assuming the ergodicity, the time average serves the purpose of evaluating the
ensemble average. The following quantities are calculated: The sublattice magnetisations
\( m_{\text{top}} = \langle \frac{1}{L^2} \sum_i S_i^z \rangle; \ i \ \forall \ \text{top layer} \), \( m_{\text{mid}} = \langle \frac{1}{L^2} \sum_i S_i^z \rangle; \ i \ \forall \ \text{middle layer} \) and \( m_{\text{tot}} = \langle \frac{1}{L^2} \sum_i S_i^z \rangle; \ i \ \forall \ \text{bottom layer} \) the total magnetisation
\( m_{\text{tot}} = (m_{\text{top}} + m_{\text{mid}} + m_{\text{bot}})/3 \), \( m_{\text{tot}} = 3m'_{\text{tot}} \) and the susceptibility \( C = L^2 \frac{J_{bb} kT}{kT} \langle (m_{\text{mid}} - \frac{1}{L^2} \sum_i S_i^z)^2 \rangle; \ i \ \forall \ \text{middle layer} \), where in all cases \( \langle ... \rangle \) stands for the time average over \( 6 \times 10^5 \) MCSS. The temperature
is measured in the unit of \( \frac{J_{bb}}{k} \).

III. Results:

The sublattice magnetisations of all three layers, the total magnetisation and the sus-
ceptibility are studied as functions of temperature. The values of \( J_{bb} = 1.0 \) and \( J_{ab} = -0.5 \)
are kept fixed throughout the study. Only the values of \( J_{aa} \) and \( D \) are varied.

What would happen for low \( J_{aa} \), say \( J_{aa} = 0.2 \)? In Fig\[2\]a the sublattice magnetisations,
total magnetisation are shown for \( J_{aa} = 0.2 \) and \( D = 0.4 \). The critical temperature
\( T_{\text{critical}} \) is also marked where all the sublattice magnetisations and the total magnetisation
vanish. Below the critical temperature, there exists a temperature, so called compensation
temperature \( (T_{\text{compensation}}) \) where the total magnetisation vanishes for nonzero values of
sublattice magnetisations of all three layers. For some other value of \( D = 0.8 \), the \( T_{\text{critical}} \) and
\( T_{\text{compensation}} \) changes, as shown in Fig\[2\]b. The critical temperature \( T_{\text{critical}} \) was mea-
sured from the position of the maximum of the susceptibility \( C \) plotted against temperature
(shown in Fig\[2\]h and Fig\[2\]i)). However, the compensation temperature was measured by
linear interpolation in the region where the total magnetisation changes sign below the criti-
cal temperature. Since, the interval \( (\Delta T) \) of temperature for cooling the system is equals to
0.05, the size of the maximum error in estimating the critical and compensation temperature
is 0.1. From Fig\[2\] it is clear that both the compensation temperature \( T_{\text{compensation}} \) and the
critical temperature \( T_{\text{critical}} \) decreases as the anisotropy \( D \) decreases.
How does the spin configuration looks like in different temperatures? For high temperature (above $T_{\text{critical}}$), each of all the sublattice magnetisations vanishes. As a result, the total magnetisation vanishes. The image plots of the spin configurations of all three layers are shown in Fig.3 for $T = 2.25$. Below the critical temperature and above the compensation temperature, say $T = 1.45$, all the sublattice magnetisation and the total magnetisation are nonzero. It is shown in Fig.4. In both cases, $D = -0.4$, $J_{aa} = 0.2$.

This compensation phenomenon can be realised as follows: if the intra layer ferromagnetic interaction strength were chosen equal in all layers and with a fixed inter layer antiferromagnetic interaction, the trilayered system would exhibit almost equal magnitude of sublattice magnetisation. However, top layer and bottom layer would show the same sign of sublattice magnetisation and middle layer would show different sign of sublattice magnetisation. As a result, the system would show the total magnetisation (essentially the sublattice magnetisation of any one of top and bottom layer) and only the critical temperature would be found. Below the critical temperature no such temperature was observed where the total magnetisation could vanish. But, if the intra layer ferromagnetic interaction strength of top and bottom layers is relatively weak in comparison to that for the middle layer, the sublattice magnetisation in top and bottom layers would be smaller in magnitude (having same sign of course) than that of the middle layer (having opposite sign). As a result, below the critical temperature, a temperature could be found where the net magnetisation vanishes. What will be the role of anisotropy $D$? For large value of $D$ with negative sign (in equation-1), will map the Blume-Capel model in spin-1/2 Ising model. Relatively, weak negative $D$ will produce a few number of $S^z = 0$. For positive $D$ the number of $S^z = 0$ will increase. So, by changing the value of anisotropy $D$, one can control the value of the magnitude of sublattice magnetisation at any fixed temperature.

The compensation phenomenon was found to disappear for larger and positive value of $D = 1.0$ and $J_{aa} = 0.2$. This is shown in Fig.5. In this case, the number of $s^z = 0$ is such that it is incapable of yielding the compensation.

What would happen if $J_{aa}$ is moderately higher, say $J_{aa} = 0.6$? In this case, for negative anisotropy $D$ no compensation was observed. However, it appears for positive anisotropy $D$, Fig.6 shows such a comparison. For $D = 1.4$, the compensation was observed (Fig.7a). The compensation was not found for $D = -1.0$ (Fig.7b). In both cases, the critical temperatures $T_{\text{critical}}$ were estimated from the positions of maxima of the susceptibilities $C$ (Fig.7c and Fig.7d).

By estimating the critical temperature from the susceptibility $C$ and the compensation temperature $T_{\text{compensation}}$ from the linear interpolation near the change of sign of total magnetisation $m_{\text{tot}}$, the comprehensive phase boundary was be obtained. Such a phase boundary was shown in Fig.8. It may be noted here that the compensation could be found only for positive values of $D$. A very narrow region bounded by the boundaries of $T_{\text{compensation}}$ and $T_{\text{critical}}$ was observed.

Can one expect to observe the compensation for very high value of $J_{aa} = 0.8$? Fig.9a and Fig.9b, show the variations of sublattice magnetisation and the total magnetisation as functions of the temperature. From these plots no compensation is observed. Only the critical temperatures can be estimated from the temperature variations of the susceptibility $C$ (shown in Fig.9c and Fig.9d). The comprehensive phase boundary (only for $T_{\text{critical}}$) was drawn and shown in Fig.10.
IV. Summary
The equilibrium properties of Blume-Capel trilayered magnet have been studied by Monte Carlo simulation with Metropolis single spin flip algorithm. The A-B-A type of trilayer is considered, where the intralayer ferromagnetic interaction strength of the middle (B say) layer is $J_{bb} = 1$. The other two layers (bottom (A) and top (A) say) have intralayer ferromagnetic interaction strength $J_{aa}$. The interlayer antiferromagnetic strength is $J_{ab}$. For fixed values of $J_{bb}=1$ and $J_{ab} = -0.5$, the sublattice magnetisation was studied as function of temperature. The critical temperature was found from the maximum of the susceptibility and the compensation temperature was determined from the linear interpolation of the two points where the total magnetisation changed sign. The critical temperature and the compensation temperature were studied as function of the anisotropy $D$ for different parameter values of the relative interaction strengths $J_{aa}/J_{bb}$, namely weak, moderate and high. For a range of values of the strength of anisotropy $D$, the weak relative interaction $J_{aa}/J_{bb} = 0.2$ shows compensation behaviours. In this range, the difference between the critical temperature and the compensation temperature is quite high. The moderate $J_{aa}/J_{bb} = 0.6$ value of relative interaction, shows compensation for positive values of the anisotropy only. In this case, the difference between the critical and compensation temperatures are very small. The compensation was not observed (in the wide range of values of $D$) for high value of $J_{aa}/J_{bb} = 0.8$.

V. Acknowledgements: Author would like to acknowledge the FRPDF grant provided by the Presidency University.
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Figure 1: The geometric structure of the system of trilayered magnetic model. Collected from I. J. L. Díaz and N. S. Branco, cond-mat:1711.10367.
Figure 2: The magnetisations of different layers and the total magnetisation are plotted against the temperature. The corresponding susceptibilities are also plotted against the temperature of the system.
Figure 3: The image plots of the values of the spins in different layers. Here, $D = -0.4$, $J_{aa} = 0.2$, $J_{bb} = 1.0$, $J_{ab} = -0.5$ and $T = 2.25$. 
Figure 4: The image plots of the values of the spins in different layers. Here, $D = -0.4$, $J_{aa} = 0.2$, $J_{bb} = 1.0$, $J_{ab} = -0.5$ and $T = 1.45$. 
Figure 5: The magnetisations of different layers and the total magnetisation are plotted against the temperature.

D=1.0, J_{aa}=0.2, J_{bb}=1.0, J_{ab}=-0.5

Figure 6: Phase diagram in the D-T plane. Here, J_{aa} = 0.2, J_{bb} = 1.0 and J_{ab} = -0.5.
Figure 7: The magnetisations of different layers and the total magnetisation are plotted against the temperature. The corresponding susceptibilities are also plotted against the temperature of the system.
Figure 8: Phase diagram in the D-T plane. Here, $J_{aa} = 0.6$, $J_{bb} = 1.0$ and $J_{ab} = -0.5$. 
Figure 9: The magnetisations of different layers and the total magnetisation are plotted against the temperature. The corresponding susceptibilities are also plotted against the temperature of the system.
Figure 10: Phase diagram in the D-T plane. Here, $J_{aa} = 0.8$, $J_{bb} = 1.0$ and $J_{ab} = -0.5$. No compensation is observed here.
