

# Monte Carlo simulations of the magnetic properties of a site-disordered Blume Capel multilayer spin-1 system

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## Abstract

We used standard Monte Carlo simulations to investigate the magnetic properties of a spin-1 Ising multilayer system composed of two non-equivalent planes A and B, where B being site-diluted. Antiferromagnetic interlayer and ferromagnetic intralayer spin couplings have been considered. Our calculations indicated the occurrence of a compensation phenomenon where the magnetization vanishes before the critical temperature. The effects of various model parameters on the system magnetic properties have been examined in detail and presented in the form of phase diagrams. The results bore some resemblance with those reported in some previous works on systems with or without site-dilution. Depending on values of the spin concentration parameter  $P$  the model displayed first- and second-order phase boundaries with the existence of a tricritical point.

## Keywords

Blume Capel model, Multilayer spins system, Site dilution, Monte Carlo method, Compensation temperature, Tricritical point.

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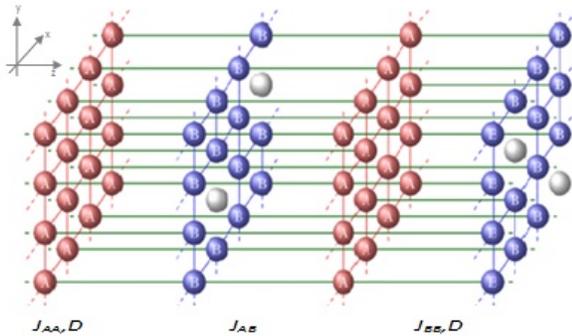
## 1. Introduction

One of the main research subjects in recent years, in the field of condensed matter and statistical mechanics, is the study of the magnetic properties of thin magnetic films with a multilayer structure [1]. As a result, magnetic multilayers present an extremely useful and wide range of magnetoelectronic phenomena, notably magnetoresistance, spin transfer torque, and interlayer exchange coupling [2]. In general, magnetic multilayers comprise alternating stacks of ferromagnetic and non-ferromagnetic spacer layers. Typical thickness of an individual layer varies from a few atomic layers (AL) to a few tens of AL. Usually, magnetic layers are composed of elemental metallic ferromagnets (Fe, Co, Ni) or alloys of them (for example, permalloy). The spacer layers may be made of any transition or noble metal; they may be paramagnetic (Cu, Ag, Au, Ru, Pd, V, etc.) or antiferromagnetic (Cr, Mn) [3]. On the other hand, multilayer magnetic systems consisting of alternating layers of different magnetic materials are of high importance due to their novel and even useful properties [4–8]. Furthermore, when a multilayer system consists of two materials with different interactions, for example, antiferromagnetic and ferromagnetic, rather unusual and interesting phase diagrams can result [5].

The investigation of ferrimagnetic materials has received considerable interest in recent decades, particularly because a number of phenomena related to these materials have great potential for technological applications [9–11]. In addition to these features, the presence of a temperature compensation is an interesting phenomenon of such layered materials. The compensation temperature ( $T_{comp}$ ) is a temperature below the critical one, for which the total magnetization is zero [12], even if the magnetization of the sublattice is not zero. In mixed spin systems, the compensation phenomenon is usually investigated. This phenomenon has been examined, especially by mean-field theory on a square [13] and hexagonal lattices [14] and by Monte Carlo simulations on a square lattice [15–17] in the mixed spin-3/2 and spin-5/2 Ising model. Certain single-spin systems, like layered magnets consisting of stacked nonequivalent ferromagnetic planes, also have been used successfully to model ferrimagnetics. A bilayer Ising system with spin-1/2 and no dilution has been examined via transfer matrix (TM) [18, 19], renormalization group (RG) [20–22], mean-field approximation (MFA) [20], and Monte Carlo (MC) simulations [20–23].

It has also been implemented in the pair approximation (PA) to investigate related systems such as Ising-Heisenberg bilayers [24, 25] and multilayers [24] with spin-1/2 and no dilution.

While site dilution is a crucial ingredient for the occurrence of a compensation point in a single spin system with an even



**Figure 1.** A schematic representation of the multilayer systems. The intralayer exchange integrals for two adjacent atoms in the same layer are  $J_{AA} > 0$  (A layer) and  $J_{BB} > 0$  (B layer). The intralayer exchange integral is  $J_{AB} < 0$ .

number of layers, the compensation effect will only be found in very specific conditions even in diluted systems, as verified by PA calculations for the Ising-Heisenberg bilayer [26] and multilayer [27], and by the Monte Carlo method for the Ising bilayer [28] and multilayer [29]. Examples of the realization and research of such bilayer [30], trilayer [31, 32] and multilayer [33–37] systems can be found in recent experimental studies. Regarding ferromagnetic bilayers with antiferromagnetic couplings, there is very little theoretical work dealing with this problem [38–41] or with a similar case of multilayers [42, 43]. The properties of some more complicated multilayer structures were also investigated [44–46].

Recently, there has been an interest in Monte Carlo simulation, of the effect of Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction and the influence of the four-spin interaction  $J_4$ , on the multilayer transition and magnetic properties of a spin-1/2 Ashkin Teller model [47], and on the critical behaviours of thin magnetic Ashkin Teller films at the special point [48, 49]. In the latest years, particular attention has been given to the theoretical and experimental study of higher order spin couplings in Ising models [50]. The spin-1 Ising model in the presence of a crystal field, called the Blume-Capel (BC) model, is one of the most studied higher spin Ising models in statistical physics. This model has been widely explored, not only due to the fundamental theoretical interest arising from the rich phase diagram it provides, but also due to the fact that variants and extensions of the model have gained application in the description of ternary fluids [51], solid-liquid-gas mixtures and binary fluids [52, 53], microemulsions [54, 55], ordering in semiconducting alloys [56] and electron conduction models [57].

In this paper, we focus on the type of multilayer systems [27, 29] with site dilution, where dilution is a necessary condition for the presence of a non-zero compensation temperature. No studies to the best of our knowledge have yet been performed on multilayer systems with site dilution in the spin-1

Ising model (Blume-Capel (BC) model). To this end, we present a study on the magnetic properties of a Blume-Capel system consisting of two types of non-equivalent planes, A and B, alternately stacked. One of the planes is randomly diluted, under the effect of the crystal field  $D$ . All intra-layer interactions are ferromagnetic, whereas inter-layer interactions are antiferromagnetic. Our objective is to determine the conditions for the occurrence of the compensation effect and the contribution of each parameter to the appearance of this effect. As a result, we carried out this study with the help of a Monte Carlo simulation based on the Metropolis algorithm [58]. In Sec. 2, we introduce our multilayer model, write down its Blume-Capel Hamiltonian, and describe the simulation method. Next, we present our results and discussion in Sec. 3. And finally, the conclusion is presented in Sec.4.

## 2. Model and simulations method

We investigate the multilayer system, in which the spins are located at the sites of simple cubic (sc) crystalline lattices. The system is composed of non-equivalent parallel monolayers (A and B) that are stacked alternately (see Figure 1). The A-planes are made up exclusively of atoms of type A, whereas the B-planes contain B-type atoms and non-magnetic impurities. Our system is defined by the conventional Blume-Capel Hamiltonian [59, 60]:

$$-\beta H = +\sum_{\langle i \in A, j \in A \rangle} K_{AA} S_i S_j + \sum_{\langle i \in A, j \in B \rangle} K_{AB} S_i S_j \varepsilon_j \quad (1)$$

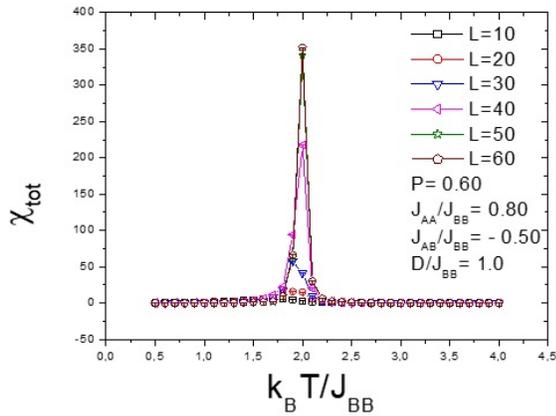
$$+ \sum_{\langle i \in B, j \in B \rangle} K_{BB} S_i S_j \varepsilon_i \varepsilon_j + \beta D \sum_{i \in A} S_i^2 + \beta D \sum_{j \in B} S_j^2 \varepsilon_j$$

where:

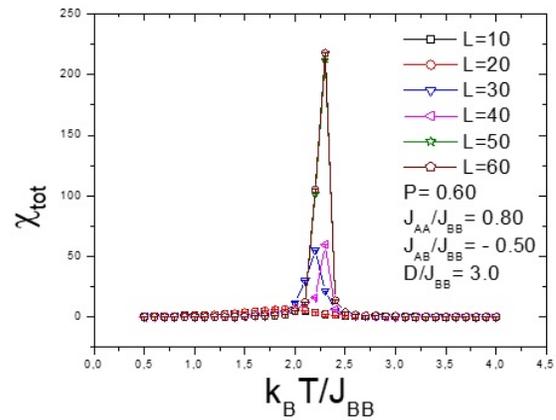
- $\langle i \in A, j \in A \rangle$  and  $\langle i \in B, j \in B \rangle$  represent the sum of all pairs of closest sites in the same layer.
- $\langle i \in A, j \in B \rangle$  are located on the closest pairs of sites in the neighboring layers.
- $S_i$  is the spin variables taking the values  $\pm 1, 0$ .
- $\beta = 1/k_B T$ ,  $T$  is the temperature and  $k_B$  is the Boltzmann constant,  $k_B = 1$  for the sake of simplicity.
- The couplings are  $K_{\gamma\tau} = \beta J_{\gamma\tau}$  where  $\gamma = A, B$  and  $\tau = A, B$  with  $K_{AA} > 0$  for an AA pair,  $K_{BB} > 0$  for a BB pair and  $K_{AB} < 0$  for an AB pair.
- The corresponding exchange integrals (see Fig. 1) are presented by:  $J_{\gamma\tau} = \beta^{-1} K_{\gamma\tau}$ , where  $\gamma = A, B$  and  $\tau = A, B$ .
- $J_{AA}$  and  $J_{BB}$  designate the intralayer nearest-neighbor bilinear exchange coupling parameters.
- $J_{AB}$ : is the interlayer bilinear interaction of nearest-neighbor spins between the layers.
- $D$ : represents the crystal field.

The site occupation operators  $\varepsilon_i$  are uncorrelated, quenched, random variables that assume the values  $\varepsilon_i = 1$  with probability  $P$  (spin concentration) or  $\varepsilon_i = 0$  with probability  $1 - P$  (spin dilution, or impurity concentration).

To simulate the Hamiltonian (1), we performed the Metropolis algorithm [58] for the Monte Carlo simulation, on cubic



**Figure 2.** The magnetic susceptibility  $\chi_{tot}$  as a function of the dimensionless temperature  $k_B T / J_{BB}$ , for  $J_{AA} / J_{BB} = 0.80$ ,  $J_{AB} / J_{BB} = -0.5$ ,  $P = 0.60$ , for the value of the crystal field  $D / J_{BB} = 1.0$ , and linear lattice sizes  $L$  ranging from 10 to 60. The error bars are not shown, as they are smaller than the symbols.



**Figure 3.** Total susceptibility  $\chi_{tot}$  as a function of the dimensionless temperature  $k_B T / J_{BB}$ , for  $J_{AA} / J_{BB} = 0.80$ ,  $J_{AB} / J_{BB} = -0.5$ ,  $P = 0.60$ , for the value of the crystal field  $D / J_{BB} = 3.0$ , and linear lattice sizes  $L$  ranging from 10 to 60. The error bars are not shown, as they are smaller than the symbols.

lattices of size  $L^3$  with periodic boundary conditions. We ran simulations for linear sizes  $L$  from 10 to 60 and for a variety of values of Hamiltonian parameters:  $0.0 < J_{AA} / J_{BB} \leq 1.0$ ,  $-1.0 \leq J_{AB} / J_{BB} < 0.0$  and  $0.0 < P \leq 1.0$ .

For each set of values chosen for the above parameters, we ran simulations for a range of temperatures near the critical point or the compensation point. Our simulations ran typically from  $10^6$  to  $3 \times 10^6$  MC steps. We discarded up to  $10^5$  steps to account for the equilibrium. When running Monte Carlo simulations, we compute some observables such as the dimensionless extensive energy  $E \equiv H / J_{BB}$ , the magnetizations of A-type atoms and B-type atoms:

$$E = - \sum_{\langle i \in A, j \in A \rangle} \left( \frac{J_{AA}}{J_{BB}} \right) S_i S_j - \sum_{\langle i \in A, j \in B \rangle} \left( \frac{J_{AB}}{J_{BB}} \right) S_i S_j \epsilon_j \quad (2)$$

$$- \sum_{\langle i \in B, j \in B \rangle} S_i S_j \epsilon_i \epsilon_j - \frac{D}{J_{BB}} \sum_{i \in A} S_i^2 - \frac{D}{J_{BB}} \sum_{j \in B} S_j^2 \epsilon_j$$

$$m_A = \frac{1}{N_A} \sum_{i \in A} S_i \quad (3)$$

$$m_B = \frac{1}{N_B} \sum_{i \in B} S_i \epsilon_i \quad (4)$$

Where  $N_A = L^3 / 2$  is the total number of A-type atoms in the system and  $N_B = p L^3 / 2$  is the number of B-type atoms. Then, the total magnetization of the system, and the magnetic susceptibilities are given respectively by:

$$m_{tot} = \frac{1}{2} (m_A + p m_B) \quad (5)$$

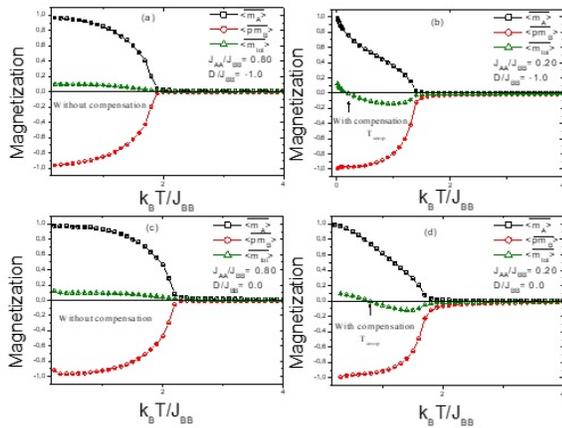
$$\chi_\tau = N_\tau K (\overline{\langle m_\tau^2 \rangle} - \langle |m_\tau| \rangle^2) \quad (6)$$

Where  $\langle \dots \rangle$  denotes the thermal average for a single disorder configuration, while we shall designate the subsequent average over disorder configurations of  $\langle \dots \rangle$  as  $\overline{\langle \dots \rangle}$ ,  $K = J_{BB} (k_B T)^{-1}$  represents the inverse dimensionless temperature, and  $\tau = A, B, tot$ . The total number of atoms in the system is:  $N_{tot} = N_A + N_B$ . The errors related to magnetization and susceptibilities were calculated by the jackknife method [61].

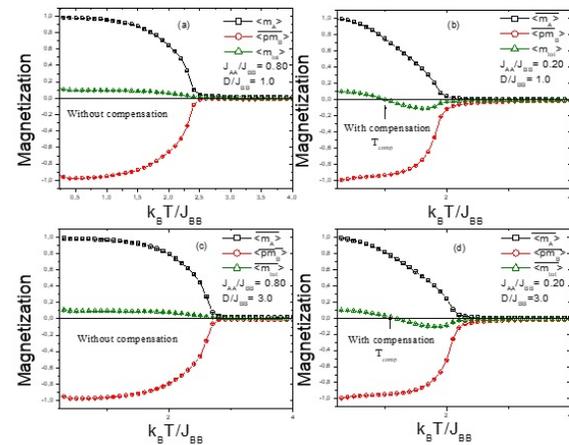
### 3. Results and discussion

We carried out our study of the magnetic behavior of multi-layer systems with site dilution, where dilution is a necessary condition for the presence of a non-zero compensation temperature, in the spin-1 Blume-Capel (BC) model by Monte Carlo simulations.

We begin our investigation by examining the temperature dependence of the total magnetic susceptibility of the system for a variety of values of the Hamiltonian parameters  $J_{AA} / J_{BB} = 0.80$ ,  $J_{AB} / J_{BB} = -0.50$ ,  $P = 0.60$ , for different system sizes  $L = 10$  to 60 and for crystal field values  $D / J_{BB} = 1.0$  in Figure 2 and  $D / J_{BB} = 3.0$  in Figure 3. The peaks of the total susceptibility increases with increasing the lateral size  $L$  of the system. These total susceptibility curves typically diverge at critical temperature  $T_c$  for infinite size  $L$ . It is clear that the critical temperatures (peak temperatures) increase with the increase of the crystal field  $D / J_{BB}$  as shown in Figures 2 and 3.



**Figure 4.** The magnetizations  $\langle m_A \rangle$ ,  $\langle pm_B \rangle$  and total magnetization  $\langle m_{tot} \rangle$  as a function of the dimensionless temperature  $k_B T / J_{BB}$  for  $P=0.80$ ,  $J_{AB}/J_{BB}=-0.5$  and  $L=60$ . For (a)  $D/J_{BB}=-1$ ,  $J_{AA}/J_{BB}=0.80$ , shows no compensation effect. (b)  $D/J_{BB}=-1$ ;  $J_{AA}/J_{BB}=0.20$ , indicates a compensation temperature  $T_{comp}$  such that  $\langle m_{tot} \rangle = 0$ , whereas (c)  $D/J_{BB}=0.0$ ;  $J_{AA}/J_{BB}=0.80$ , has no compensating effect, and (d)  $D/J_{BB}=0.0$ ;  $J_{AA}/J_{BB} = 0.20$ , shows a compensation temperature  $T_{comp}$ . The error bars are smaller than the symbols.



**Figure 5.** The magnetizations  $\langle m_A \rangle$ ,  $\langle pm_B \rangle$ , and total magnetization  $\langle m_{tot} \rangle$  as a function of the dimensionless temperature  $k_B T / J_{BB}$  for  $P=0.80$ ,  $J_{AB}/J_{BB}=-0.5$  and  $L=60$ . For (a)  $D/J_{BB}=1.0$ ;  $J_{AA}/J_{BB}=0.80$ , shows no compensation effect. (b)  $D/J_{BB}=1.0$ ;  $J_{AA}/J_{BB}=0.20$ , indicates a compensation temperature  $T_{comp}$  such that  $\langle m_{tot} \rangle = 0$ , whereas (c)  $D/J_{BB}=3.0$ ;  $J_{AA}/J_{BB}=0.80$ , has no compensating effect, and (d)  $D/J_{BB}=3.0$ ;  $J_{AA}/J_{BB} = 0.20$ , shows a compensation temperature  $T_{comp}$ . The error bars are smaller than the symbols.

Our aim is to provide a detailed account of the regions in parameter space where the compensation phenomenon is present or absent, for several crystal field values  $D/J_{BB}$  and under the effect of the intralayer bilinear exchange coupling parameter of nearest-neighbor spins between the layers  $J_{AA}/J_{BB}$ . Then, the compensation point for each set of Hamiltonian parameters is defined as the temperature  $T_{comp}$  where the total magnetization is zero  $\langle m_{tot} \rangle = 0$ , while  $\langle m_A \rangle \neq 0$  and  $\langle pm_B \rangle \neq 0$ . The critical point is computed as the temperature where all magnetizations disappear simultaneously.

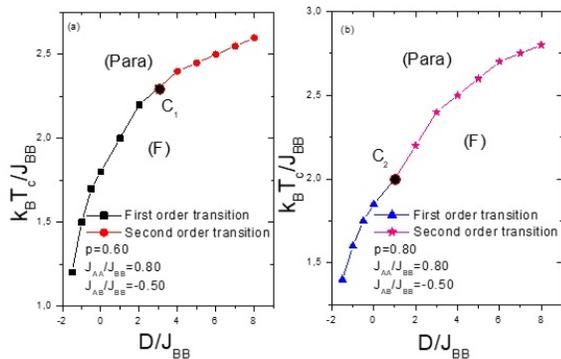
To investigate the effect of  $D/J_{BB}$  and  $J_{AA}/J_{BB}$  in the behavior of the system, we fixed values for  $J_{AB}/J_{BB} = -0.5$ ,  $P = 0.80$  and  $L = 60$ , and plotted the magnetization  $\langle m_A \rangle$  and  $\langle pm_B \rangle$  and total magnetization  $\langle m_{tot} \rangle$  versus dimensionless temperature  $k_B T / J_{BB}$  as seen in Figures 4(a-d) and 5(a-d).

The total magnetization curve  $m_{tot}$  in Figure 4(b,d) and Figure 5(b,d), shows a clear sign of the compensation phenomenon, where we have observed a compensation temperature  $T_{comp}$  such as  $\langle m_{tot} \rangle = 0$  and  $\langle m_A \rangle, \langle pm_B \rangle \neq 0$ , for  $\{D/J_{BB} = -1.0, D/J_{BB} = 0.0 \text{ and } J_{AA}/J_{BB} = 0.20\}$  (see Figure 4(a,d)), and for  $\{D/J_{BB} = 1.0, D/J_{BB} = 3.0 \text{ and } J_{AA}/J_{BB} = 0.20\}$  (see Figure 5(a,d)). Therefore, this compensation temperature increases with increasing of the crystal field  $D/J_{BB}$ . For  $J_{AA}/J_{BB} = 0.80$ , on the other hand, we did not find a compensating effect (Figure 4(a,c) and Figure 5(a,c)). This can be understood by the fact that when the

intralayer bilinear exchange coupling parameter increases, the compensation phenomena disappears. This behavior is comparable to that found in multilayers with spin-1/2 and dilution [29], and trilayers [62] with spin-1/2 and no dilution. The nature of the phase transition is established by the discontinuity and continuity of the order parameters. Consequently, a second-order phase transition occurs.

In Figure 6(a,b), we showed the phase diagrams in the  $(k_B T_c / J_{BB}, D/J_{BB})$  plane for  $J_{AA}/J_{BB} = 0.80$ ,  $J_{AB}/J_{BB} = -0.50$  and  $L = 60$ , under the influence of  $P$ .

Figure 6a shows the case where  $P = 0.60$ ; it is seen that the disordered paramagnetic (Para) where  $\langle S \rangle = 0$  and ordered ferromagnetic (F) where  $\langle S \rangle \neq 0$  phases are separated by the first-order phase transition line, for negative values of  $D/J_{BB} = -1.5$  to  $3.0$ . Then while, from  $D/J_{BB} = 3$  to  $8$ , the transition becomes second order. The discontinuous and continuous phase transition lines cross at a tricritical point, which is denoted by the bold point  $(C_1)$ , whose coordinates are  $(D/J_{BB} = 3.0 \text{ and } T_c = 2.3 \text{ at } J_{AA}/J_{BB} = 0.80)$ . We have also noticed that when the values of the crystal field  $D/J_{BB}$  increase, the critical temperature  $k_B T_c / J_{BB}$  also increases. Furthermore, by increasing the value of spin concentration to  $P = 0.80$ , Figure 6b also shows that there is a first order phase transition between the (Para) and (F) phases. In addition, from  $D/J_{BB} = 2.0$  to  $8.0$ , the transition is of the second order. These two lines meet at a tricritical point  $(C_2)$  of coordinates  $(D/J_{BB} = 1.0 \text{ and } T_c = 2.0 \text{ at } J_{AA}/J_{BB} = 0.80)$ . It can be seen



**Figure 6.** Phase diagram of the critical temperature as a function of the crystal field  $D/J_{BB}$  for  $J_{AA}/J_{BB}=0.80$ ,  $J_{AB}/J_{BB}=-0.50$  and  $L=60$ . Figure (a), for  $P=0.60$ . whereas figure (b),  $P=0.80$ .

that when we increase the value of  $P$ , the tricritical point shifts towards lower values of its coordinates  $k_B T_C / J_{BB}$  and  $D / J_{BB}$ . We also notice that the critical line is characterized by an increasing temperature  $k_B T_C / J_{BB}$  increases with increasing of the crystal field  $D / J_{BB}$ .

#### 4. Conclusion

In summary, we have studied the magnetic behavior of a spin-1 Blume Capel multilayer model. The system consists of two kinds of non-equivalent planes, A and B, where only the B layers are site-randomly diluted, under the effect of the crystal field  $D / J_{BB}$ . The study was performed using Monte Carlo simulations based on the Metropolis algorithm. The occurrence of a compensation phenomenon was checked, and the compensation temperatures were determined for different crystal field values. Therefore, the magnetization curves show a second order phase transition behavior. The phase diagrams in the  $(k_B T_C / J_{BB}, D / J_{BB})$  plane show a variety of phase transitions, including first and second-order phase transitions meeting at a tricritical points that depends on spin dilution  $P$ .

#### Conflict of interest statement:

The authors declare that they have no conflict of interest.

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