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# Monte Carlo studies of critical phenomena in mixed spin-3/2 and spin-5/2 Ising model on square lattice

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We used a Monte Carlo simulation to analize the magnetic behavior of Ising model of mixed spins $S_i^A = \pm 3/2, \pm 1/2$ and $\sigma_j^B = \pm 5/2, \pm 3/2, \pm 1/2$, on a square lattice. Were studied the possible critical phenomena that may emerge in the region around the multiphase point $(D/|J_1| = -3, J_2/|J_1| = 1)$ and the dependence of the phase diagrams with the intensities of the anisotropy field of single ion $(D/|J_1|)$ and the ferromagnetic coupling of exchange spin $S_i^A$ $(J_2/|J_1|)$. The system displays first order phase transitions in a certain range of the parameters of the Hamiltonian, which depend on $D/|J_1|$ and $|J_2/|J_1|$. In the plane $(D/|J_1|, k_BT/|J_1|)$, the decrease of $|D/|J_1||$, implies that the critical temperature, $T_c$, increases and the first order transition temperature, $T_t$, decreases. In the plane $(J_2/|J_1|, k_BT/|J_1|)$, $T_c$ increases with the increasing of $J_2/|J_1|$, while that $T_t$ decreases.

*Keywords:* Ising system; single-ion anisotropy; Monte Carlo simulation; critical temperatures; first-order transitions.

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## 1. Introduction

Actually, the mixed Ising models are a valuable theoretical tool for the description and understanding of the thermomagnetic behavior of various magnetic molecular systems, which can exhibit ferrimagnetic properties [1]. Besides, the mixed-spin Ising models belong to the most interesting extensions of the standard spin-1/2 Ising model, which may display more diverse critical behaviour compared with their single-spin counterparts. Continuously from the molecular magnetism have been working on the design and synthesis of new magnetic molecular materials [2], since that through of specific controls in these processes, such as the sustitution of a metal by other, is open the possibility of arising new magnetic properties [3, 4]. The unusual magnetic properties of the complex ferrimagnetic systems, require that the design of the processes in the creation of new materials, must be optimal, therefore is required the understanding of the mechanisms that originate these properties, specifically exchange interactions between different molecules that form the compound, and that can affect phenomena such as transition and compensation temperatures [5]. Some of molecular magnets are formed by two kinds of magnetic atoms, alternating in a regular lattice [3, 6–10] and with the possibility to display several important physical phenomena, such as magnetoelastic transitions [11,12], compensation temperatures [13, 14], first order phase transitions [15–18], tricritical points [15, 19, 20] and reentrant phenomena [21–23]. Note that from the experimental point of view, various physical systems, such as classic fluids, solid $^3H_e$, lipid bilayers and rare gases [24], have been described with mixed Ising models of multispin interactions [25] and random crystal field; and also, experimental results in amorphous ferromagnetic oxides, where $F_e^{3+}$ ions are present [26]. It has been demonstrated that Ising systems of mixed spins, are interesting models for the study of the ferrimagnetic ordering and the rich variety of multicritical phenomena presented by the molecular magnets, for this have been used various methods and lattice structures. T. Kaneyoshi by using mean field theory, investigated the longitudinal and transverse thermal variation of the magnetization in a ferroelectric nanoparticle, simulated with a two-dimensional hexagonal structure, through a transverse Ising model [27]; Y. Lin *et al* by using two-dimensional lattice Ising, they simulated a field programmable gate array (FPGA), which is a valuable contribution to the scientific computing platforms, especially in the field of the Monte Carlo simulation method [28]; Strecka *et al*, solved as an exact form the spin system $(1/2, 1)$ on two totally frustrated triangular lattices, finding reentrant phase transitions with two or three successive critical points and a spontaneous ordering system [23]; Taherkhani *et al* using renormalization group theory demonstrated for anisotropic Ising two-dimensional models, in triangular, square and hexagonal lattices, that the magnitude of the spin coupling interaction with anisotropic ferromagnetic characteristics does not change the values of the critical exponent [29] and the magnetic properties of Ising spin system $(1/2, S)$, on a decorated Bethe lattice were calculated exactly in a previous work by J. Strecka and C. Ekiz [30]. On the other hand, high-spin systems, such as $(3/2, 5/2)$ and $(5/2, 2)$ [31–36], are the most important and used for analysis of the thermomagnetic behavior of many cooperative physical systems. For the study of these systems have been considered coupling of ferromagnetic exchange, external magnetic fields and crystalline fields originating the anisotropy of the lattice, which affect the magnetic properties of these mixed models, as influence on its molecular magnetism. Preliminary studies based on mean-field methods suggest that the ferrimagnetic Ising spin model $(3/2, 5/2)$ presents an interesting magnetic behavior [11, 12, 16, 17, 37], and would be interesting to solve it with nonperturbative methods such as Monte Carlo model [38]. Of this system have been investigated the compensation temperatures induced by single ion anisotropy and external longitudinal fields, on square and cubic lattices [39]; the phase diagrams for different ground state interactions in the Hamiltonian and the magnetic behavior by Monte Carlo methods [40, 41]; the phase diagrams and internal energy on a hexagonal lattice with interlayer coupling, using effective field theory with correlations [22]; up to two compensation points in a Bethe lattice by exact recursion relations [16]; transitions of first and second order in a two-fold Cayley tree, through the method of exact recursion relations [11]; phase transitions and dynamic temperature compensation, with a mean field approximation [12]. G. Wei *et al* [38], made a Monte Carlo study on the critical phenomena around a multiphase point in the phase diagram of the ground state of mixed Ising spin $(1, 3/2)$, achieving interesting results for the model $J - D_A - D_B$, especially first order phase transitions, and compared with those reported by JW Tucker, via variational theory of cluster pair approximation [42], demonstrating more complete results of the investigated system. On the other hand, De La Espriella and Buendía [40, 41] calculated energy diagrams of the ground state and the magnetic behavior of the system of Ising mixed spin $S_i^A$=$\pm 3/2, \pm 1/2$ and $\sigma_j^B$ = $\pm 5/2, \pm 3/2, \pm 1/2$, on a square lattice, under the model $J_1 - J_2 - D$. The ground state diagram of this model, presents several points where more than two phases can coexist, as in the case of $(D/|J_1| = -3, J_2/|J_1| = 1)$ in the plano $(D/|J_1|, J_2/|J_1|)$(Fig. 1 of [41]). The main objective of our research is to analyze the various critical phenomena that can emerge around of the multiphase point. We studied the effects of the anisotropy of simple ion $D/|J_1|$ and exchange energy $J_2/|J_1|$, on the magnetization and the specific heat of the system. Additionally, Sec. 2 describes the model and the Monte Carlo simulation, Sec. 3 presents and discusses our results, and finally the conclussions in Sec. 4.

## 2. Methodology

The model studied is a mixed Ising ferrimagnet with spins $3/2$ and $5/2$, alternating on a square lattice of side $L = 80$. The interaction Hamiltonian of the system is defined as:

$$H = -J_1 \sum_{i,j\epsilon<nn>} S_i^A \sigma_j^B - J_2 \sum_{i,k\epsilon<nnn>} S_i^A S_k^A - D\sum_{i\epsilon A}(S_i^A)^2 - D\sum_{j\epsilon B}(\sigma_j^B)^2 \quad (1)$$

where $S_i^A$= $\pm 3/2, \pm 1/2$ and $\sigma_j^B$ = $\pm 5/2, \pm 3/2, \pm 1/2$, are the spins on the sites of the sublattices $A$ and $B$, respectively. $J_1$ is the exchange interaction between pairs of spins to nearest neighbors, $J_2$ is the exchange parameter between pairs of spins next nearest neighbors of the sublattice $A$, and $D$ is the crystal field, it causes anisotropy of the system. The first sum is performed over all pairs of spins with nearest neighbor interaction, *i.e.* between sites with spins $S_i^A = 3/2$ and $\sigma_j^B = 5/2$, the second sum runs over all pairs of spins with next nearest neighbors interaction of spins $S_i^A$, and sums $\sum_i$ and $\sum_j$ are performed on all sites of spins of the sublattices $A$ and $B$, respectively. We choose a ferrimagnetic coupling to nearest neighbors, $J_1 < 0$, and we take periodic boundary conditions. All variables in the Hamiltonian are in units of energy.

We applied standard importance-sampling algorithms to simulate the model. Data were generated with 50.000 Monte Carlo steps per site after discarding the first 10.000 steps [43]. We define $\beta = 1/k_BT$. Our program calculates the internal energy $\langle H\rangle$ , the specific heat per site,

$$C = \frac{\beta^2}{L^2}[\langle H^2\rangle - \langle H\rangle^2] \quad (2)$$

and the sublattice magnetizations per site, defined as

$$M_A = \frac{2}{L^2}\langle\sum_{i\epsilon A} S_i^A\rangle \quad , \quad M_B = \frac{2}{L^2}\langle\sum_{j\epsilon B} \sigma_j^B\rangle \quad (3)$$

and the total magnetization per site $M_T = (M_A + M_B)/2$.

## 3. Results and discussions

It was found that the phase diagrams of the ground state of the mixed model Ising, are useful for the study of phase diagrams at finite temperature, are also a useful tool to identify regions in which the models could present an interesting magnetic behavior, especially around the points where more than two phases can coexist, in addition they can check the reliability of the simulation results [38]. According to Fig. 1 of the Ref. 41, around the point $(D/|J_1| = -3, J_2/|J_1| = 1)$, important critical phenomena can emerge as first order phase transitions, where their behavior can be judged by considering the presence of discontinuities in the magnetization and energy, as well as hysteresis loops [44]. We will focus on this multiphase point, considering the effects of parameters $D/|J_1|$ and $J_2/|J_1|$ on first order transition temperature $(T_t)$, second order $(T_c)$ and the magnetic properties of the system. For all calculations $J_1 < 0$, the critical points are estimated by the location of the peaks of the specific heat and $(T_t)$ by discontinuities in the magnetization [44]. Initially the values of $J_2/|J_1|$ are fixed, then do the inverse case.

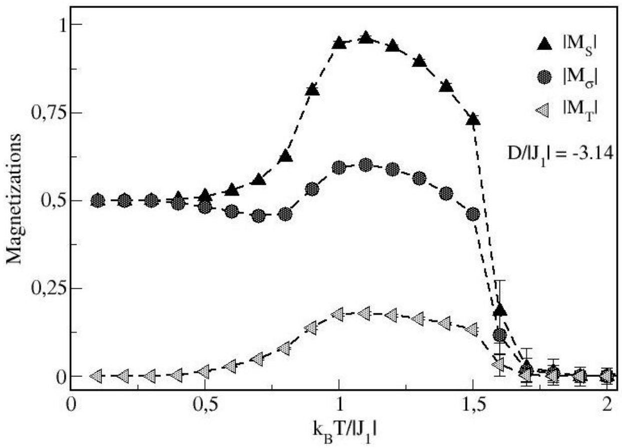


FIGURE 1. Magnetization of the system, $|M_S|$, $|M_\sigma|$ and $|M_T|$ as functions of temperature for $J_2/|J_1| = 0.975$ and $D/|J_1| = -3.14$.

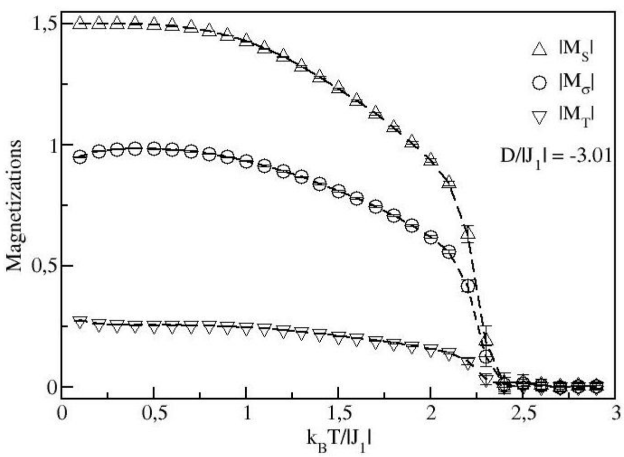


FIGURE 2. Magnetization of the system, $|M_S|$, $|M_\sigma|$ and $|M_T|$ as functions of temperature for $J_2/|J_1| = 0.975$ y $D/|J_1| = -3.01$.

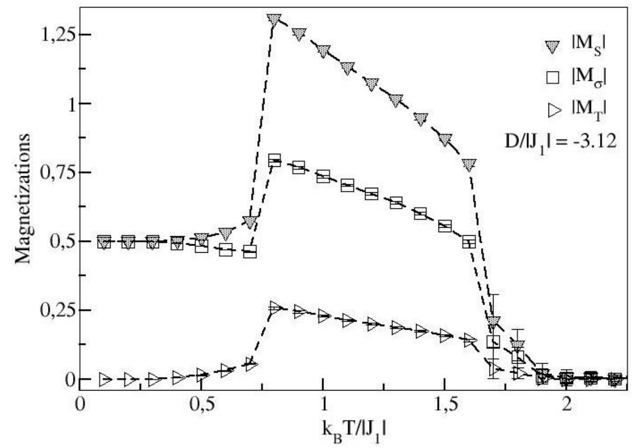


FIGURE 3. Magnetization of the system, $|M_S|$, $|M_\sigma|$ and $|M_T|$ as functions of temperature for $J_2/|J_1| = 0.975$ y $D/|J_1| = -3.12$.

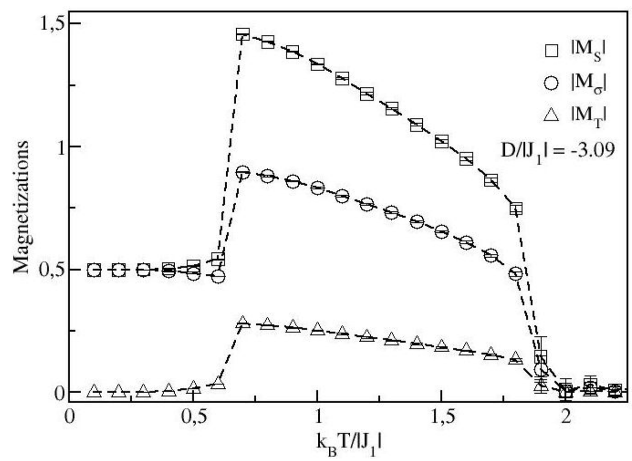


FIGURE 4. Magnetization of the system, $|M_S|$, $|M_\sigma|$ and $|M_T|$ as functions of temperature for $J_2/|J_1| = 0.975$ y $D/|J_1| = -3.09$.

### 3.1. Effect of single ion anisotropy $D$

We fix the exchange parameter $J_2/|J_1| = 0.975$ and vary the crystal field in the range $-3.14 \leq D/|J_1| \leq -3.01$, these are points very close to the multiphase point ($D/|J_1| = -3$, $J_2/|J_1| = 1$). Figures 1 and 2 exhibit the magnetizations of the sublattices and the total lattice as functions of temperature, for extreme values of the selected range, $D = -3.14$ and $D = -3.01$. In these cases, only second order phase transitions occur; the system goes from a ferrimagnetic phase to a paramagnetic phase when $T > T_c$. Due to the ferromagnetic coupling ($J_2 > 0$) exerted on the spins type $S_i^A$, is seen in Fig. 2 that the sublattice $A$ is more ordered that the sublattice $B$. In addition, the decrease of the single ion anisotropy module, leads to an increase in the critical temperature of the system ($T_c$) as the maximum of the magnetizations disappear, and experience higher values for $T = 0K$.

As the magnitude of the single ion anisotropy decreases to $D < -3.01$, appear interesting phenomena such as first order phase transitions, as reflected in the discontinuous behavior of the magnetization curves of ferrimagnetic system [44], in Figs. 3, 4 and 5. For $D/|J_1| = -3.12$, $D/|J_1| = -3.09$ and $D/|J_1| = -3.03$, the system present non-continuos phase transitions in the magnetization, and as $|D/|J_1||$ decreases, the first order transition temperature, ($T_t$), decreases and critical temperature increases.

With the increasing temperature, to the first order phase transition ($T \leq T_t$), in Figs. 3, 4 and 5 shows that the magnetic moments are moving towards higher values, while for ($T > T_t$) transiting towards lower values, which is reflected in the values of the magnetization. This indicates that the first order phase transitions ferri-ferri, occur when the crystal field module is a little larger as that $D/|J_1| = -3$. For values close to $D/|J_1| \geq -3$ the phenomenon of the first order phase transitions is not found, as seen in Fig. 6, which exhibits the behavior of the magnetization as a function of temperature, when $D/|J_1| = -2.99$. The behavior of the specific heat of the system is reflected in Fig. 7. Addition-

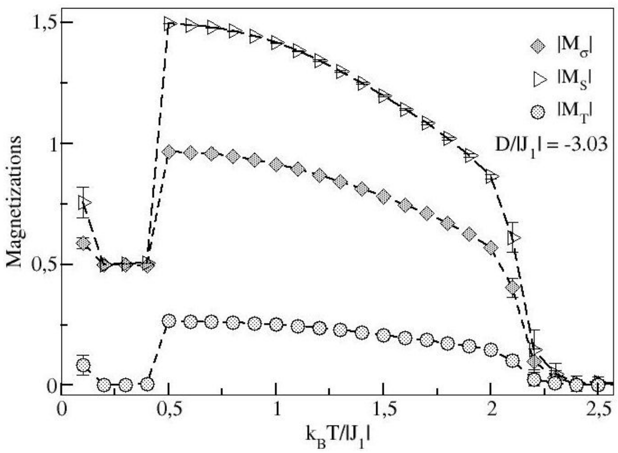


FIGURE 5. Magnetization of the system, $|M_S|$, $|M_\sigma|$ and $|M_T|$ as functions of temperature for $J_2/|J_1| = 0.975$ y $D/|J_1| = -3.03$.

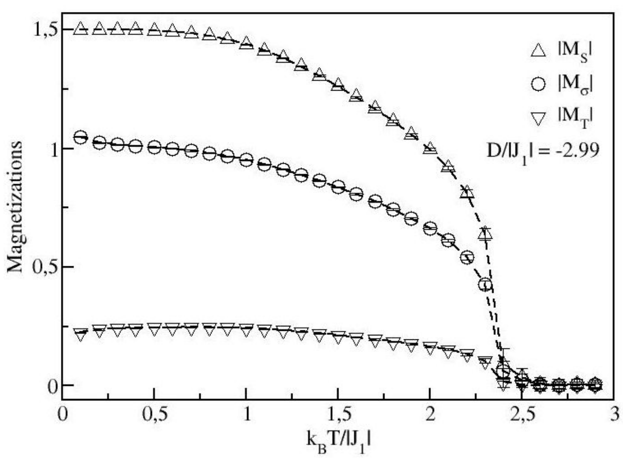


FIGURE 6. Magnetization of the system, $|M_S|$, $|M_\sigma|$ and $|M_T|$ as functions of temperature for $J_2/|J_1| = 0.975$ y $D/|J_1| = -2.99$.

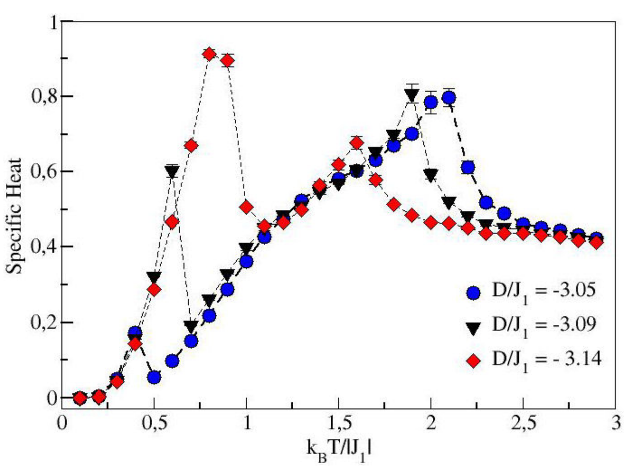


FIGURE 7. Specific heat per spin as functions of temperature for different values of $D/|J_1|$ y $J_2/|J_1| = 0.975$.

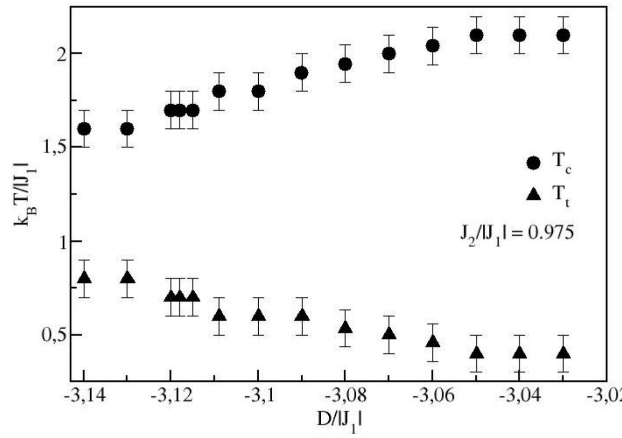


FIGURE 8. Detailed study of the transition temperatures as functions of the ionic anisotropy of the total lattice, with $J_2/|J_1| = 0.975$.

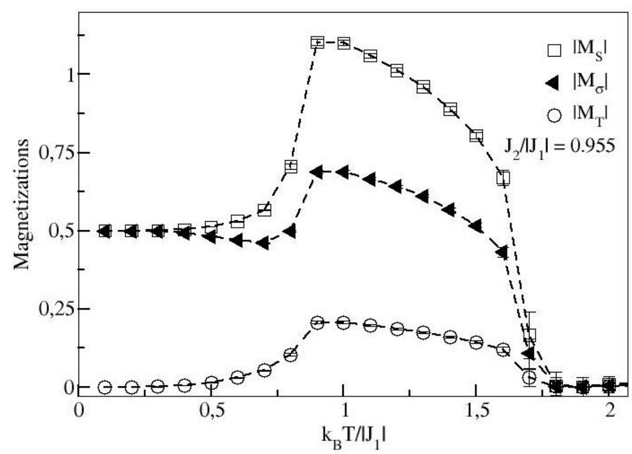


FIGURE 9. Magnetization of the system, $|M_S|$, $|M_\sigma|$ and $|M_T|$ as functions of temperature for $J_2/|J_1| = 0.955$ y $D/|J_1| = -3.1$.

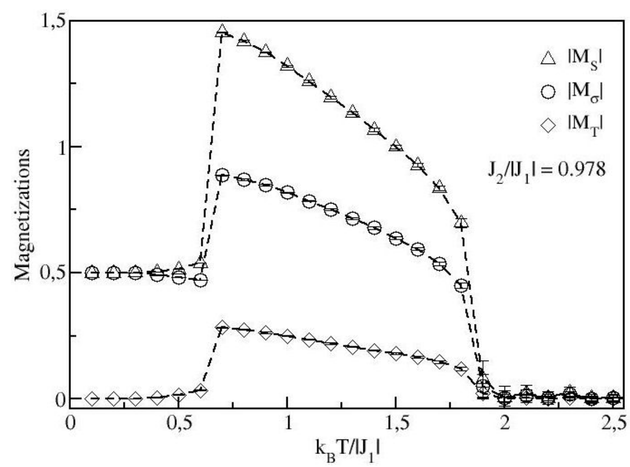


FIGURE 10. Magnetization of the system, $|M_S|$, $|M_\sigma|$ and $|M_T|$ as functions of temperature for $J_2/|J_1| = 0.978$ y $D/|J_1| = -3.1$.

ally, are observed secondary peaks to $T \lesssim 0.75$, where the system undergoes noncontinuous phase transitions in $T = T_t$. It is possible that the secondary peaks arise from the thermal rearrangement of the spins of $B$ sublattice [41]. A detailed study of the transition temperatures as functions of the single ion anisotropy is shown in Fig. 8. The curve

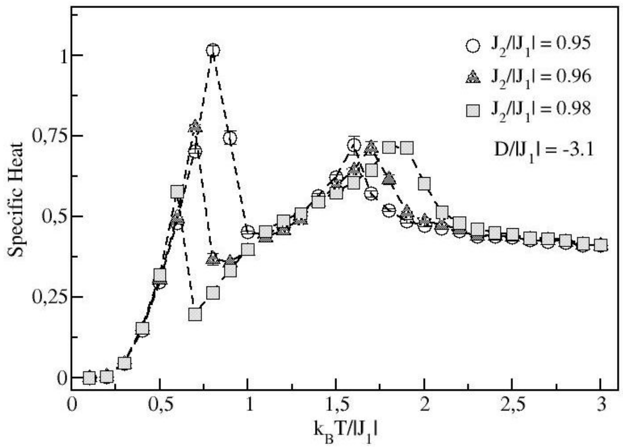


FIGURE 11. Specific heat per spin as functions of temperature for different values of $J_2/|J_1|$ with $D/|J_1| = -3.1$.

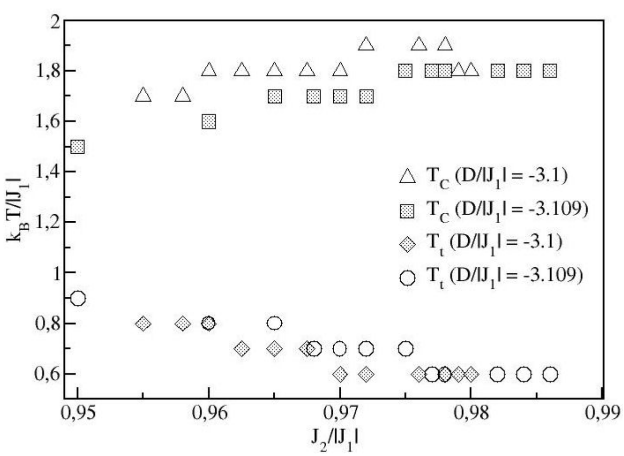


FIGURE 12. Detailed study of the transition temperatures as functions of the $J_2/|J_1|$, with $D/|J_1| = -3.1$ and $D/|J_1| = -3.109$.

$T_t$ separates the first order phase transitions ferri-ferri, while the curve $T_c$ separates the second order phase transition ferri-para. When $|D/|J_1||$ decreases $T_t$ and $T_c$ tend to constant values.

### 3.2. Effect of the exchange interaction $J_2/|J_1|$

We analyze the influence of the exchange interaction $J_2/|J_1|$ on the Ising spin ferrimagnetic $S_i^A$= $3/2$ and $\sigma_j^B$ = $5/2$ in the range $0.95 \leqslant J_2/|J_1| \leqslant 0.98$, considering fixed values $D/|J_1| = -3.1$ and $D/|J_1| = -3.109$ for the crystal field. The Figs. 9 and 10 show first order phase transitions, in the abrupt jump of the curves of the total magnetization and sublattices, around the temperature range $0.6 \lesssim T \lesssim 0.8$. By increasing the ferromagnetic coupling of the spins type $S_i^A$, the first order transition temperature, $T_t$, decreases, and once appears $T_t$ the system magnetizations decrease toward the second order transition at $T = T_c$. On the other hand, the increase of the exchange parameter implies an increase in the critical temperature of the system. Figure 11 shows that the maxima of the specific heat is transferred to the region of high temperatures, as the parameter $J_2/|J_1|$ grows positively, *i.e*, the critical temperature increases. All curves exhibit a second non-critical peak, right where the ferrimagnetic model undergoes the noncontinuous phase transition $(0.6 \lesssim T \lesssim 0.8)$, which are independent of the lattice size; this characteristic was reported by Selke and Oitma in ferrimagnetic Ising models on the square lattices, as a result of interaction of the system with the crystal field [45]. The critical behavior of the system as a function of $J_2/|J_1|$ is summarized in Fig. 12, for $D/|J_1| = -3.1$ and $D/|J_1| = -3.109$. It is evident that the increase of $|D/|J_1||$, causes an decrease in the critical temperature, and as the ferromagnetic exchange energy, $J_2/|J_1|$, increases on the spins of the sublattice $A$, the transition temperatures $T_t$ and $T_c$ tends to a constant value.

## 4. Conclusion

We investigate the critical behavior of a mixed spins ferrimagnetic Ising $S_i^A$= $\pm 3/2, \pm 1/2$ and $\sigma_j^B$ = $\pm 5/2, \pm 3/2, \pm 1/2$, on a square lattice around the point $(D/|J_1| = -3, J_2/|J_1| = 1)$, using the Monte Carlo method and periodic boundary conditions. For the fixed value $J_2/|J_1| = 0.975$ and the value range $-3.14 \leq D/|J_1| \leq -3.01$, the system exhibits first order phase transitions ferri-ferri, as for fixed values $D/|J_1| = -3.1$ and $D/|J_1| = -3.109$ of the crystal field, in the range $0.95 \leq J_2/|J_1| \leq 0.98$. First order phase transitions ferri-ferri, occur when the crystal field module is a bit larger than $D/|J_1| = -3$, and for values close to $D/|J_1| \geq -3$ no phenomenon of first order phase transitions was found. With the decrease of $|D/|J_1||$, the $T_t$ decreases to a constant value, while the $T_c$ is increased to a limit value. When $|D/|J_1||$ is fixed, the increase of $J_2/|J_1|$ produces a decrease of $T_t$, and an increase in $T_c$, to a constant value. The limit values reaching both transition temperatures are independent of the value of $|D/|J_1||$. The study on the spin system $(3/2, 5/2)$, yielded qualitatively similar results to those reported in the Refs. 45 and 38, for specific heat non-critical peak and first order phase transitions, respectively. It also confirms that the ground state diagrams are not only useful to check the reliability of the results at finite temperatures, but are valuable for identifying multiphase points and study the magnetic behavior of the system in their neighborhoods, as in our case.

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