Mixed spin-1 and spin-2 Ising model: study of the ground states

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Abstract

We calculate ground state configurations of a mixed Ising model on a square lattice where spins $S^A_i = \pm 2, \pm 1, 0$ in one A sublattice are in alternating sites with spins $\sigma^B_j = \pm 1, 0$, located on the other B sublattice. The Hamiltonian of the system includes nearest-neighbors interactions between the $S^A_i$ and $\sigma^B_j$ spins, next-nearest-neighbors interactions between the $S^A_i$ spins, and between the $\sigma^B_j$ spins, single-ion anisotropy, and an external magnetic field.

1. Introduction

Many of the novel magnetic materials that are been synthesized for industrial or academic interest, are of the type $A_pB_{1-p}$, where $A$ and $B$ are compounds with different spins, arranged in alternate sites of a crystal, frequently experimenting a repulsive interaction between them. As an example we can mention the so-called prussian blue analogs, superlattices of Fe$_3$O$_4$ or Mn$_3$O$_4$ [1, 2]. The relevance of these systems relays on their ability of changing their magnetic properties just by the change of one compound for another, creating the enticingly possibility of designing materials ‘a la carte’. These compounds have many potential applications in the area of thermomagnetic and magneto-optical recording, as well as been an ideal source to study a variety of critical phenomena [3–5]. Despite their relative simplicity, mixed spin Ising models have proven to be very useful to study the magnetic and critical properties of these materials [6–10]. Mixed Ising models have been studied by mean-field approaches, and numerical simulations [11–14]. Experimental results of amorphous ferrimagnetic oxides where Fe$^{II}$ ions are present, have been analyzed by mixed Ising models [15].

Theoretical studies predict that several of these systems present compensation temperatures ($T_{comp}$), i.e. temperatures below the critical one at which the total magnetization is zero but the sublattice magnetizations are not, this phenomenon is possible due to the different spin values on the sublattices, and the antiferromagnetic interaction between them. Generally, in the $T < T_{comp}$ range one of the sublattices is more ordered, such that it maintains its saturation value at $T = 0$, at relatively high temperatures, while the disorder in the other sublattice is due to the fact that its spins tend to change of direction by effects of some specific parameter in the Hamiltonian. Here the magnetizations have opposite signs but the cancelation is still incomplete due to the residual magnetization that exists as a result of ferrimagnetic interaction to first neighbors in the lattice, which tend to align the nearby spins in opposite directions. When the system increases its temperature, residual magnetization may change its direction, i.e., at this moment the thermal energy prevails and many spins tend to change its orientation, until that at $T = T_{comp}$, the sublattices are compensated, i.e., $|M_A| = |M_B|$ and $|M_T| = 0$ [16, 17], magnetization reversal, photoinduced magnetizations, etc. [18–21].

Most of these phenomena have been observed experimentally. Experiments show that Fe$_3$O$_4$ and Mn$_3$O$_4$ superlattices [22], presents compensation points. Studies by Kageyama et al on the magnetic properties of nickel (II) formate dihydrate compound Ni(HCOO)$_2$·2H$_2$O, show that in addition to magnetization reversal, this system presents compensation points [23]. Compounds where magnetic atoms Fe$^{II}$ and Fe$^{III}$ alternate regularly on a layered honeycomb lattice, such as AFe$^{II}$Fe$^{III}$C$_2$O$_4$$_3$ ($A = N - C_nH_{2n+1}$)$_x$, $n = 3 - 5$ [24–27], and Fe$^{II}$Fe$^{III}$ bimetallic oxalates, present ferrimagnetic ordering and compensation temperatures, properties that

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have been reproduced by mixed Ising system solved by effective-field theories [28]. Other interesting properties such as surface magnetoelastic coupling and surface magnetic anisotropy, have been studied experimentally in some magnetic thin films, formed by multilayer spin systems [29–31]. Also experimental results indicate that the presence of longitudinal magnetic fields plays an important role in the properties of mixed spin magnetic systems [32–34].

Higher spin systems present diverse and interesting physical phenomena, such as the spin-1 Ising system with bilinear and biquadratic interactions that presents magnetic relaxation [35], first-order transition [36], and tricritical behavior in the presence of a transverse crystal field [37], possible reentrant phenomenon due to the competitive effects between exchange interactions in the Hamiltonian [38], dynamic compensation temperature in an oscillating external magnetic field on alternate layers of a hexagonal lattice [39], as well as reentrant and double reentrant phenomena [40] and the existence of tricritical points when the system is under the effect of random crystal field and surface exchange interactions [41]. The spin-2 Ising model have been investigated on a bilayer square lattice [42], and in the presence of a longitudinal crystal field within the framework of mean-field theory and effective-field theory [43], among others. The mixing of higher spins compounds presents even more interesting properties. As an example we can mention mixed spin-1–spin2 systems. Masrour et al investigated hysteresis and compensation behaviors on hexagonal Ising nano wire core–shell structure in these model [44], Korkmaz and Temizer analyzed the dynamic compensation temperature in an oscillating field on alternate layers of a hexagonal lattice [45]. Additionally this system undergoes second-and first-order phase transition, tricritical point and reentrant behavior [46, 47]. It is worth mentioning previous work of Zhang et al on the magnetization, compensation point, phase diagram, internal energy and specific heat of the spin 1–spin2 model [48]; as well as investigations of Keskin et al on the dynamic phase transition temperatures and dynamic phase diagrams of this system [49], and its the magnetic properties in the presence with different anisotropies reported by Wei et al [50].

An important step for the comprehension of these mixed models is the calculation of their ground state. The ground state diagrams are very useful to understand the low temperature behavior of the system [11, 51–55], and to test the behavior of the techniques used in their simulation. Also, these diagrams can be used to locate regions of the phase parameter where an interesting magnetic behavior can emerge. Depending on the spins that are mixed and the interactions taken into account, these diagrams can be quite complex, showing high degeneration, and points where several magnetic phases can coexist. Tsuchima et al confirm that the ground state of the spin-3/2 Ising model have a fourfold degeneracy [56], and Dublenych obtained the conditions of nonexistence of the intermediate nonuniform phases for the spin-1 Ising model on unfrustrated lattices, through the construction of ground state diagrams of classical spin models [57]. De La Espriella et al have calculated the ground state for the mixed 3/2-5/2 and the 2-5/2 on a square lattices [58, 59].

The purpose of this paper is to calculate the energies of the spin2–spin1 mixed Ising system at zero temperature. The ground state diagrams are calculated exactly by enumerating all the possible states of the unit cell of the system in a square lattice and numerically calculating their energy. The paper is organized as follows. In section 2 we define the model and explain how the ground state diagrams are calculated. In the subsections therein we present the ground state diagrams for different combinations of parameters in the Hamiltonian. The conclusions are presented in section 4.

2. Model and method

We consider a mixed Ising spin-1 and spin-2 system, where spins are located on alternating sites of a square lattice. Spins $S_A^i = \pm 2$, $\pm 1$, 0 and $S_B^j = \pm 1, 0$ are on the sites of the interpenetrating sublattices $A$ and $B$, respectively. The system is described by the Hamiltonian

$$
\mathcal{H} = -J_A \sum_{\langle mn \rangle} S_A^m S_A^n - J_B \sum_{\langle mm \rangle} S_A^m S_B^n - J_B \sum_{\langle mm \rangle} S_B^m S_B^n - D_1 \sum_i (S_A^i)^2 - D_2 \sum_j (S_B^j)^2 - h \sum_i S_A^i - h \sum_j S_B^j,
$$

where $\langle mn \rangle$ and $\langle mm \rangle$ are the next and next-nearest neighbors, respectively, $J_A$, $J_B$ and $J_C$ are the exchange bilinear interactions, $D_1$ and $D_2$ are the crystal fields. $h$ is an external magnetic field. All in energy units. For simplicity, in some cases we will consider a single-ion anisotropy constant, $D_1 = D_2 = D$, in the understanding that it represents the average crystal field felt by the entire lattice.

A conjecture of Luttinger and Tisza [60] establishes that for a system of spins with next-nearest interactions, the minimum energy configuration is invariant under any translation by twice the lattice spacing. It was later
proven that this conjecture can also be applied to systems with next-nearest interactions [61]. According with this, for Hamiltonians translationally invariant, as the one described by equation (1), the state of minimum energy can be obtained from the $2 \times 2$ unitary cell, that for the present system is of the form, $S \sigma$.

Taking into account rotational symmetry, for the spin-1–spin-2 system this cell has $3^2 \times 5^2 = 225$ configurations. Which one of them is the ground state depends on the value of the parameters in the Hamiltonian. Many of these configurations are degenerated.

To construct the ground states we calculate numerically the energy of all the possible configurations of the unitary cell ($225$) for the different set of parameters and select the ones with the minimum energy. In the limiting case where some of the parameters are very large it is relatively easy to decide which are the configurations with the lowest energy. In the region where the parameters are small we have to be very careful and calculate the energy of all the configurations obtained by making very small changes in the values of the parameters. The equations of the boundaries between the regions of the phase diagram are calculated analytically by pairwise equating the ground state energies of the limiting regions. Due to the complexity of the Hamiltonian, we are going to discuss separately the ground states for several models that contain different combinations of parameters. These models are going to be labeled by the parameters in the Hamiltonian that are different from zero.

3. Results and discussions

3.1. The $J_1$ model

This model has only interactions between spins $S$ and $\sigma$ that are nearest-neighbors on the lattice. All other interactions in the Hamiltonian in equation (1) are neglected. As expected, the phase diagram in this case is very simple and the ground state is highly degenerate. Figure 1 shows the two regions that make up the diagram, a ferromagnetic one when $J_1 > 0$ and a ferrimagnetic one when $J_1 < 0$. The ground state energy has the same expression in both phases, $E_0 = -8|J_1|$. The coexistence line separating the two magnetic states is $J_1 = 0$.

![Figure 1. Ground state diagram for the $J_1$ model. The energy of the ground state appears in each of the regions.](image)

3.2. The $J_1 - h$ model

This model has only interactions between spins $S$ and $\sigma$ that are nearest-neighbors on the lattice and an external field $h$. All other interactions in the Hamiltonian given by 1 are neglected. The phase diagram consists of four regions as indicated in the figure 2. The regions I and II are ferromagnetics, while the regions III and IV are ferrimagnetics. Note that when a magnetic field is present each one of the two regions in figure 1 is split in two. The ground states, their energies, and the equation of the coexistence lines are shown in tables 1 and 2, respectively. The phase diagram is symmetric under the change $h \rightarrow -h$.

3.3. The $J_1 - D - h$ model

This model has interactions between spins $S$ and $\sigma$ that are nearest-neighbors on the lattice, external field $h$, and an average crystal field $D$ that is the same in all the sites. All other interactions in the Hamiltonian given by 1 are neglected. We consider separately the cases, $J_1 > 0$ and $J_1 < 0$, since the topology of the phase diagram strongly

3
depends on the sign of $J_1$. We define the dimensionless quantities, $D' D/|J_0|$ and $h' h/|J_0|$, and calculate the diagrams in the $D' - h'$ space.

3.3.1. The ferromagnetic $J_1 - D - h$ model ($J_1 > 0$)
The ground state diagram is shown in figure 3. It has five different regions separated by six coexisting lines. We observe that $D$ cause the appearance of two points where several phases coexist: $h' = 0, D' = -1$ and $h' = 0, D' = -2/3$, where three and four phases coincide, respectively.

At zero, and probably at very low temperatures, the phases I, II, III and V are ferromagnetic, while in phase IV the larger, negative values of $D$ prevail making the ground state consisting of spins zero. The ground state spin configurations and their energies are shown in table 3, and the equations of the coexistence lines are in table 4.

3.3.2. The ferrimagnetic $J_1 - D - h$ model ($J_1 < 0$)
The ground state diagram is shown in figure 4. The ground state configurations and their energies are shown in table 5. The diagram is way more complex than the one for the ferromagnetic case. Now it has twelve regions separated by twenty coexistence lines whose equations are given in table 6. The ground states in regions I, VII, VIII and XII are ferromagnetic, the III and V are ferrimagnetic (taking in consideration only nn alignments). In regions II, VI and XI only the $\sigma$ spins are zero, while in region IX only the $S$ spins are zero. In region X all the spins are zero. The diagram has five points where the ground state has a degeneration of three, and four points, $(h', D') = (3, -1), (1, -1), (-1, -1), (-3, -1), (-3, -1)$, where the degeneration is four. This particular phase diagram, that we include for completitude, has already been published by Deviren et al [46].
Figure 3. Ground state diagram for the $J_1 - D - h$ model with $J_1 > 0$. The ground states and their energies are shown in Table 3 and the equations of the coexistence lines are indicated in the Table 4.

Table 3. Spin configurations and ground states energies $J_1 - D - h$ model with $J_1 > 0$ (corresponding to Figure 3).

| $a_1^x a_2^x$ | $a_1^y a_2^y$ | Energy | Region |
|----------------|----------------|--------|--------|
| ++ ++          | ++ ++          | $-8h - 10D - 6h$ | I      |
| +1 +2          | +1 +2          | $-8h - 10D + 6h$ | II     |
| -2 -1          | +1 -1          | $-4h - 4D - 4h$ | III    |
| 0 0            | 0 0            | 0      | IV     |
| +1 +1          | +1 +1          | $-4h - 4D - 4h$ | V      |

Table 4. Coexistence curves $J_1 - D - h$ model with $J_1 > 0$ (corresponding to Figure 3).

| Phases | Line | $b'$ range | $D'$ range |
|--------|------|------------|------------|
| I–II   | $h' = 0$ | $h' = 0$ | $D' \geq -2/3$ |
| II–III | $D' = (1/3)h' - (2/3)$ | $h' \leq 0$ | $D' \leq -2/3$ |
| III–IV | $D' = h' - 1$ | $h' \leq 0$ | $D' \leq -1$ |
| III–V  | $h' = 0$ | $h' = 0$ | $-1 \leq D' \leq -2/3$ |
| IV–V   | $D' = -(1/3)h' - (2/3)$ | $h' \geq 0$ | $D' \leq -1$ |
| I–V    | $D' = -(1/3)h' - (2/3)$ | $h' \geq 0$ | $D' \leq -2/3$ |

Figure 4. Ground state diagram for the $J_1 - D - h$ model with $J_1 < 0$. The ground states and their energies are shown in Table 5 and the equations of the coexistence lines are indicated in the Table 6.
Table 5. Spin configurations and ground states energies $J_1 - D - h$ model with $J_1 < 0$ (corresponding to figure 4).

| $\hat{J}_1$ | $\hat{S}_1$ | Energy                  | Region |
|------------|------------|------------------------|--------|
| $+2 \, +1$ | $+1 \, +2$ | $-8J_1 - 10D - 6h$     | I      |
| $+2 \, 0$  | $+2 \, -2$ | $-8D - 4h$             | II     |
| $-1 \, +2$ | $-1 \, +2$ | $8J_1 - 10D - 2h$      | III    |
| $-2 \, 0$  | $-2 \, -2$ | $8J_1 - 10D + 2h$      | V      |
| $-1 \, 0$  | $-1 \, 0$  | $-8D + 4h$             | VI     |
| $0 \, 0$   | $0 \, 0$   | $-8J_1 - 10D + 6h$     | VII    |
| $0 \, 0$   | $2 \, 0$   | $-4J_1 - 4D + 4h$      | VIII   |
| $0 \, -1$  | $0 \, -1$  | $-2D + 2h$             | IX     |
| $0 \, 1$   | $0 \, 1$   | $-2J - 2h$             | XI     |
| $0 \, 1$   | $1 \, +1$  | $-4J_1 - 4D - 4h$      | XII    |

Table 6. Coexistence curves $J_1 - D - h$ model with $J_1 < 0$ (corresponding to figure 4).

| Phases | Line | $h'$ range | $D'$ range |
|--------|------|------------|------------|
| I–II   | $D' = -h' + 4$ | $4 \leq h' \leq 5$ | $-1 \leq D' \leq 0$ |
| I–III  | $h' = 4$      | $h' = 4$      | $D' \geq 0$    |
| II–III | $D' = h' + 4$ | $3 \leq h' \leq 4$ | $-1 \leq D' \leq 0$ |
| III–IV | $D' = -(1/3)h' - (2/3)$ | $0 \leq h' \leq 1$ | $-1 \leq D' \leq -2/3$ |
| III–V  | $h' = 0$      | $h' = 0$      | $D' \geq -2/3$ |
| IV–V   | $D' = (1/3)h' - (2/3)$ | $-1 \leq h' \leq 0$ | $-1 \leq D' \leq -2/3$ |
| V–VI   | $D' = -h' - 4$ | $-4 \leq h' \leq -3$ | $-1 \leq D' \leq 0$ |
| V–VII  | $h' = -4$     | $h' = -4$     | $D' \geq 0$    |
| VI–VII | $D' = h' + 4$ | $-5 \leq h' \leq -4$ | $-1 \leq D' \leq 0$ |
| VII–VIII| $D' = (1/3)h' + (2/3)$ | $h' \geq 0$ | $D' \leq -1$ |
| VII–IX | $D' = -1$     | $-5 \leq h' \leq -3$ | $D' \leq -1$ |
| VIII–IX| $D' = h' + 2$ | $-5 \leq h' \leq -3$ | $D' \leq -1$ |
| V–IX   | $D' = -1$     | $-3 \leq h' \leq -1$ | $D' \leq -1$ |
| IX–X   | $D' = h'$     | $-3 \leq h' \leq -1$ | $D' \leq -1$ |
| IV–X   | $D' = -1$     | $-1 \leq h' \leq 1$ | $D' \leq -1$ |
| X–XI   | $D' = h'$     | $h' \geq 1$     | $D' \leq -1$ |
| III–XI | $D' = -1$     | $1 \leq h' \leq 3$ | $D' \leq -1$ |
| IV–XI  | $D' = h'$     | $h' \geq 3$     | $D' \leq -1$ |
| II–XII | $D' = -1$     | $3 \leq h' \leq 5$ | $D' = -1$ |
| I–II   | $D' = -(1/3)h' + (2/3)$ | $h' \geq 0$ | $D' \leq -1$ |

3.4. The $J_1 - J_2 - D$ model

This model has interactions between spins $S$ and $\sigma$ that are nearest-neighbors on the lattice, between the $S$ spins that are next nearest neighbors, and an average crystal field $D$ that is the same in all the sites. All other interactions in the Hamiltonian in equation (1) are neglected. We define $J'_1 = J_2 / |J_1|$, $D' = D / |J_1|$. The phase diagram is shown in figure 5, its topology is independent on the sign of $J_1$. The ground state configurations and their energies are shown in table 7. Since $h = 0$ all the states are invariant under a global inversion of the spins. The diagram is highly asymmetrical and has seven regions, separated by eleven coexistence lines whose equations are given in table 8. There is one point where five regions coexist, $(h' = 0, D' = -1)$. 
Notice that there is a region of the parameter space where the competing effect of the $J_2$ interaction, and the negative values of $D$ that favor the zero spins, are such that the ground state can change by just making a very small change in one of the parameters. This occurs for relative small values of $J_2$ and $D < 0$.

### 3.5. The $J_1 - J_2 - D - h$ model

This model has interactions between spins $S$ and $\sigma$ that are nearest-neighbors on the lattice, between the $S$ spins that are next-nearest neighbors, an average crystal field $D$ that is the same in all the sites, and an external field $h$. Only the $J_2$ parameter in equation (1) is zero. We define $J'_2 = J_2 / |J_1|$, $D' = D / |J_1|$, $h' = h / |J_1|$, and choose $|J_1| = 1$. In this case we analyze separately the ferromagnetic and ferrimagnetic cases when $D' < 0$.

#### 3.5.1. The $J_1 - J_2 - D - h$ model with ferromagnetic ordering ($J_1 > 0$, and $D' = +1$)

The ground state diagram is shown in figure 6. The ground state configurations and their energies are shown in table 9. The diagram has four regions separated by four coexistence lines given in table 10. There is one point...
Table 8. Coexistence curves $J - J_2 - D$ model with $|h'| = 1$ (corresponding to figure 5).

| Phases | Line | $J_2'$ range | $D'$ range |
|--------|------|--------------|------------|
| I–II   | $J_2' = -(3/2)D' - 1$ | $-1 < J_2' < 0$ | $-2/3 < D' < 0$ |
| I–III  | $J_2' = -2D' - 4/3$ | $0 < J_2' < 4/3$ | $-4/3 < D' < -2/3$ |
| I–IV   | $J_2' = -(5/2)D' - 2$ | $J_2' > 4/3$ | $D' < -4/3$ |
| I–VII  | $J_2' = -1$ | $J_2' = -1$ | $D' > 0$ |
| II–III | $J_2' = -3D' - 2$ | $-4/5 < J_2' < 0$ | $-2/3 < D' < -2/5$ |
| II–VI  | $J_2' = -(1/3)D' - 1$ | $-1 < J_2' < -4/5$ | $-2/5 < D' < 0$ |
| III–IV | $J_2' = -4D' - 4$ | $-4/3 < J_2' < 4/3$ | $-4/3 < D' < -2/3$ |
| III–VI | $J_2' = 2D'$ | $-4/3 < J_2' < -4/5$ | $-2/3 < D' < -2/5$ |
| IV–V   | $J_2' = 2D'$ | $J_2' < -4/3$ | $D' < -2/3$ |
| V–VI   | $J_2' = (1/2)D' - 1$ | $-4/3 < J_2' < -1$ | $-2/3 < D' < 0$ |
| V–VII  | $D' = 0$ | $J_2' < -1$ | $D' = 0$ |

Figure 6. Ground state diagram for the $J_1 - J_2 - D - h$ model with $J_1 = 1$ and $D' = 1$. The ground states and their energies are shown in table 9 and the equations of the coexistence lines are indicated in the table 10.

Table 9. Spin configurations and ground states energies $J_1 - J_2 - D - h$ model with $J_1 = 1$ and $D' = 1$ (corresponding to figure 6).

| $\sigma_1^z \sigma_2^z$ | Energy | Region |
|-------------------------|---------|--------|
| +2 +1                   | $-8J_1 - 4J_2 - 10D - 6h$ | I      |
| +1 +2                   | $-8J_1 - 4J_2 - 10D + 6h$ | II     |
| -1 -2                   | $4J_1 - 10D + 2h$          | III    |
| +2 -1                   | $-8J_1 - 4J_2 - 10D + 6h$ | II     |
| +1 -2                   | $4J_1 - 10D - 2h$          | IV     |
| -1 +2                   | $4J_1 - 10D + 2h$          | III    |
| +2 +1                   | $4J_1 - 10D - 2h$          | IV     |

Table 10. Coexistence curves $J_1 - J_2 - D - h$ model with $J_1 = 1$ and $D' = 1$ (corresponding to figure 6).

| Phases | Line | $J_2'$ range | $h'$ range |
|--------|------|--------------|------------|
| I–II   | $h' = 0$ | $J_2' < -1$ | $h' = 0$ |
| I–IV   | $J_2' = -(1/2)h' - 1$ | $J_2' < -1$ | $h' > 0$ |
| II–III | $J_2' = (1/2)h' - 1$ | $J_2' < -1$ | $h' < 0$ |
| III–IV | $h' = 0$ | $J_2' < -1$ | $h' = 0$ |
where the degeneration of the ground state is four, the degeneracy is $\frac{\hbar J_1}{\hbar J_1 \pm 1}$.

As expected the diagram is symmetric under the change $\hbar \rightarrow -\hbar$.

### 3.5.2. The $J_1 - J_2 - D - h$ model with ferrimagnetic ordering ($J_1 < 0$, and $D' = +1$)

The ground state diagram is shown in figure 7. The ground state configurations and their energies are shown in table 11. The diagram has four regions separated by four coexistence lines given in table 12. Again the diagram is symmetric under the change $\hbar \rightarrow -\hbar$.

### 3.6. The $J_1 - D_1 - D_2$ model

In this section we are going to explore the ground state diagram when there are different crystal fields on each sublattice. This model has interactions between spins $S$ and $\sigma$ that are nearest-neighbors on the lattice, and a crystal fields $D_1$ and $D_2$ applied over the $S$ and $\sigma$ sublattice, respectively. All the other interactions in the Hamiltonian in equation (1) are taken as zero. We analyze both, the ferromagnetic ($J_1 > 0$) case and the ferrimagnetic one ($J_1 < 0$). The ground state diagram is shown in figure 8. The ground state configurations and their energies are shown in table 13, for the ferro and the ferrimagnetic cases. The diagram has five regions separated by seven coexistence lines given in table 14. The existence of different crystal fields make the diagram highly asymmetric. As expected, in region IV, where the $D$ are large and negative, the ground state has all the spins equal to zero.

| $J_{1}^{F}$ | $J_{2}^{F}$ | Energy | Region |
|------------|------------|--------|--------|
| $+1$       | $-1$       | $8h - 2J_1 - 10D - 2h$ | I      |
| $+1$       | $+1$       | $8h - 2J_1 - 10D + 2h$ | II     |
| $-1$       | $+1$       | $4h - 10D - 2h$ | III    |

Table 11. Spin configurations and ground states energies $J_1 - J_2 - D - h$ model with $J_1 = -1$ and $D' = 1$ (corresponding to figure 7).

| Phases | Line | $J_{1}^{F}$ range | $h'$ range |
|--------|------|------------------|------------|
| I–II   | $h' = 0$ | $J_{1}^{F} \geq -1$ | $h' = 0$  |
| I–IV   | $J_{1}^{F} = -1$ | $J_{2}^{F} = -1$ | $h' \geq 0$ |
| II–III | $J_{1}^{F} = -1$ | $J_{2}^{F} = -1$ | $h' < 0$  |
| III–IV | $h' = 0$ | $J_{1}^{F} \leq -1$ | $h' = 0$  |

Table 12. Coexistence curves $J_1 - J_2 - D - h$ model with $J_1 = -1$ and $D' = 1$ (corresponding to figure 7).

where the degeneration of the ground state is four, the ($h' = 0, J_{1}^{F} = -1$). As expected the diagram is symmetric under the change $\hbar \rightarrow -\hbar$.

3.5.2. The $J_1 - J_2 - D - h$ model with ferrimagnetic ordering ($J_1 < 0$, and $D' = +1$)

The ground state diagram is shown in figure 7. The ground state configurations and their energies are shown in table 11. The diagram has four regions separated by four coexistence lines given in table 12. Again the diagram is symmetric under the change $\hbar \rightarrow -\hbar$.

3.6. The $J_1 - D_1 - D_2$ model

In this section we are going to explore the ground state diagram when there are different crystal fields on each sublattice. This model has interactions between spins $S$ and $\sigma$ that are nearest-neighbors on the lattice, and a crystal fields $D_1$ and $D_2$ applied over the $S$ and $\sigma$ sublattice, respectively. All the other interactions in the Hamiltonian in equation (1) are taken as zero. We analyze both, the ferromagnetic ($J_1 > 0$) case and the ferrimagnetic one ($J_1 < 0$). The ground state diagram is shown in figure 8. The ground state configurations and their energies are shown in table 13, for the ferro and the ferrimagnetic cases. The diagram has five regions separated by seven coexistence lines given in table 14. The existence of different crystal fields make the diagram highly asymmetric. As expected, in region IV, where the $D$ are large and negative, the ground state has all the spins equal to zero.
3.7. The $J_1 - J_2 - D_1 - D_2$ model

In this section we calculate the ground state diagram for a model that includes interactions between the $S$ and $\sigma$ spins nearest-neighbors on the lattice, the $S$ spins next nearest neighbors on the lattice, and different crystal fields for each sublattice. Only the parameters $J_3$ and $h$ in the Hamiltonian given by 1 is zero. We study both cases: ferromagnetic and ferrimagnetic interactions between the $S$ and the $\sigma$ spins. We are doing this study by fixing one of the values of the crystal field and changing the other.

Table 13. Spin configurations and ground states energies $J_1 - D_1 - D_2$ model with $|J_1| = 1$ (corresponding to figure 8).

| $\sigma_1^A$ | $\sigma_1^B$ | $\sigma_2^A$ | $\sigma_2^B$ | $\sigma_1^A$ $\sigma_1^B$ | Energy | Region |
|----------|----------|----------|----------|-----------------|--------|--------|
| $\pm 2$  | $\pm 1$  | $\pm 1$  | $\pm 1$  | $\pm 1$ $\pm 1$ | $h_1 > 0$ | $-8|J_1| - 8D_1 - 2D_2$ | I |
| $\pm 1$  | $\pm 1$  | $\pm 1$  | $\pm 1$  | $\pm 1$ $\pm 1$ | $h_1 < 0$ | $-4|J_1| - 2D_1 - 2D_2$ | II |
| $\pm 1$  | $\pm 1$  | $\pm 1$  | $\pm 1$  | $\pm 1$ $\pm 1$ | $h_1 < 0$ | $-2D_2$ | III |
| $0$      | $0$      | $0$      | $0$      | $0$ $0$          | $h_1 > 0$ | 0 | IV |
| $\pm 2$  | $\pm 2$  | $\pm 2$  | $\pm 2$  | $\pm 2$ $\pm 2$ | $h_1 > 0$ | $-8D_1$ | V |

Table 14. Coexistence curves $J_1 - D_1 - D_2$ model with $|J_1| = 1$ (corresponding to figure 8).

| Phases | Line | $D_1$ range | $D_2$ range |
|-------|------|-------------|-------------|
| I–II  | $D_1 = -2/3$ | $D_1 < -2/3$ | $D_2 < -4/3$ |
| I–IV  | $D_1 = -4D_1 + 4$ | $-2/3 \leq D_1 \leq 0$ | $-4 \leq D_2 \leq -4/3$ |
| I–V   | $D_1 = -4$ | $D_1 \geq 0$ | $D_2 = -4$ |
| II–III| $D_2 = -2$ | $D_2 = -2$ | $D_2 \geq 0$ |
| II–IV | $D_2 = -D_2 - 2$ | $-2 \leq D_1 \leq -2/3$ | $-4/3 \leq D_2 \leq 0$ |
| III–IV| $D_2 = 0$ | $D_2 \leq -2$ | $D_2 = 0$ |
| IV–V  | $D_2 = 0$ | $D_2 = 0$ | $D_2 \leq -4$ |

Figure 8. Ground state diagram for the $J_1 - D_1 - D_2$ model with $|J_1| = 1$. The ground states and their energies are shown in table 13 and the equations of the coexistence lines are indicated in the table 14. We consider $D_1' = D_1/|J_1|$ and $D_2' = D_2/|J_1|$. 
3.7.1. The $J_{1} - J_{2} - D_{1} - D_{2}$ model

In this case we take the value of $\Delta = D_{1}$ and present the phase diagram in the $\Delta - \Delta$ plane. The ground state diagram is shown in figure 9, it is the same for both, $J_{1} > 0$ and $J_{1} < 0$. The ground state configurations and their energies are shown in table 15, for the ferro and the ferrimagnetic cases. The diagram has three regions separated by three coexistence lines given in table 16. Notice that after including the $J_{2}$ interaction the case where all the spins are zero is not present in the ground state diagram. This diagram is relatively simple because $D_{1}$ (that affects the $S$ spins that can take more values) is fixed, and $D_{2}$ only affects the spins zero of the sublattice $B$.

3.7.2. The $J_{1} - J_{2} - D_{1} - D_{2}$ model

Now we fix $D_{1} = 1$ and present the phase diagram in the $\Delta - \Delta$ plane. The ground state diagram is shown in figure 10, it is the same for both, $J_{1} > 0$ and $J_{1} < 0$. The ground state configurations and their energies are shown in table 17, for the ferro and the ferrimagnetic cases. The diagram has eight regions separated by thirteen coexistence lines given in table 18. Again after including the $J_{2}$ term interaction the case where all the spins are zero is not present in the ground state diagram. Notice that this diagram is way more complex than the previous one, where we fixed $D_{1}$, this is because the higher value of the spins aligned with the $D_{1}$ field. There are several points where the ground state is degenerate, in particular at the point $(\Delta' = 0, \Delta'' = -1)$, five ground states have

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**Table 15. Spin configurations and ground states energies**

$J_{1} - J_{2} - D_{1} - D_{2}$ model with $|J_{1}| = 1$ and $D_{1}' = 1$ (corresponding to figure 9).

| $s_{1}^{1} s_{2}^{1}$ | $s_{1}^{2} s_{2}^{2}$ | $J_{1}$ | Energy | Region |
|-----------------|-----------------|--------|--------|--------|
| $\pm 2 \pm 1$   | $\pm 1 \pm 2$   | $J_{1} > 0$ | $-8|J_{1}| - 4J_{2} - 8D_{1} - 2D_{2}$ | I   |
| $\pm 1 \pm 1$   | $\pm 1 \pm 1$   | $J_{1} < 0$ | $4J_{2} - 8D_{1}$ | II  |
| $\pm 1 \pm 1$   | $\pm 1 \pm 1$   | $J_{1} > 0$ | $4J_{2} - 8D_{1} - D_{2}$ | III |

**Table 16. Coexistence curves $J_{1} - J_{2} - D_{1} - D_{2}$ model with $|J_{1}| = 1$ and $D_{1}' = 1$ (corresponding to figure 9).**

| Phases | Line | $D_{1}'$ range | $J_{1}'$ range |
|--------|------|----------------|----------------|
| I-II   | $J_{1}' = -(1/4)D_{1}' - 1$ | $D_{1}' \leq 0$ | $J_{1}' \geq -1$ |
| I-III  | $J_{1}' = -1$ | $D_{1}' \geq 0$ | $J_{1}' \leq -1$ |
| II-III | $D_{1}' = 0$ | $D_{1}' = 0$ | $J_{1}' \leq -1$ |

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Figure 9. Ground state diagram for the $J_{1} - J_{2} - D_{1} - D_{2}$ model with $|J_{1}| = 1$ and $D_{1}' = 1$. The ground states and their energies are shown in table 15 and the equations of the coexistence lines are indicated in the table 16. We consider the dimensionless quantities $D_{1}' = D_{2}'/|J_{1}|$ and $J_{2}' = J_{2}/|J_{1}|$. 

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Table 15. Spin configurations and ground states energies

$J_{1} - J_{2} - D_{1} - D_{2}$ model with $|J_{1}| = 1$ and $D_{1}' = 1$ (corresponding to figure 9).

| $s_{1}^{1} s_{2}^{1}$ | $s_{1}^{2} s_{2}^{2}$ | $J_{1}$ | Energy | Region |
|-----------------|-----------------|--------|--------|--------|
| $\pm 2 \pm 1$   | $\pm 1 \pm 2$   | $J_{1} > 0$ | $-8|J_{1}| - 4J_{2} - 8D_{1} - 2D_{2}$ | I   |
| $\pm 1 \pm 1$   | $\pm 1 \pm 1$   | $J_{1} < 0$ | $4J_{2} - 8D_{1}$ | II  |
| $\pm 1 \pm 1$   | $\pm 1 \pm 1$   | $J_{1} > 0$ | $4J_{2} - 8D_{1} - D_{2}$ | III |

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Table 16. Coexistence curves $J_{1} - J_{2} - D_{1} - D_{2}$ model with $|J_{1}| = 1$ and $D_{1}' = 1$ (corresponding to figure 9).

| Phases | Line | $D_{1}'$ range | $J_{1}'$ range |
|--------|------|----------------|----------------|
| I-II   | $J_{1}' = -(1/4)D_{1}' - 1$ | $D_{1}' \leq 0$ | $J_{1}' \geq -1$ |
| I-III  | $J_{1}' = -1$ | $D_{1}' \geq 0$ | $J_{1}' \leq -1$ |
| II-III | $D_{1}' = 0$ | $D_{1}' = 0$ | $J_{1}' \leq -1$ |

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3.7.1. The $J_{1} - J_{2} - D_{1} - D_{2}$ model ($|J_{1}| = 1$, $D_{1}' = +1$)

In this case we take the value of $D_{1}' = 1$ and present the phase diagram in the $J_{1}' - D_{1}'$ plane. The ground state diagram is shown in figure 9, it is the same for both, $J_{1} > 0$ and $J_{1} < 0$. The ground state configurations and their energies are shown in table 15, for the ferro and the ferrimagnetic cases. The diagram has three regions separated by three coexistence lines given in table 16. Notice that after including the $J_{2}$ interaction the case where all the spins are zero is not present in the ground state diagram. This diagram is relatively simple because $D_{1}'$ (that affects the $S$ spins that can take more values) is fixed, and $D_{2}'$ only affects the spins zero of the sublattice $B$.

3.7.2. The $J_{1} - J_{2} - D_{1} - D_{2}$ model ($|J_{1}| = 1$, $D_{1}' = +1$)

Now we fix $D_{1}' = 1$ and present the phase diagram in the $J_{1}' - D_{1}'$ plane. The ground state diagram is shown in figure 10, it is the same for both, $J_{1} > 0$ and $J_{1} < 0$. The ground state configurations and their energies are shown in table 17, for the ferro and the ferrimagnetic cases. The diagram has eight regions separated by thirteen coexistence lines given in table 18. Again after including the $J_{2}$ term interaction the case where all the spins are zero is not present in the ground state diagram. Notice that this diagram is way more complex than the previous one, where we fixed $D_{1}$, this is because the higher value of the spins aligned with the $D_{1}$ field. There are several points where the ground state is degenerate, in particular at the point $(D' = 0, \Delta'' = -1)$, five ground states have
the same energy. Notice that this diagram is considerably more complicated than the previous one, figure 9, because, as we already mentioned, $D'_1$ is a more relevant interaction that $D'_2$ since it affects the $S$ spins that can take more values. As in figure 5, there is a region of the parameter space where the ground state can change just by making a very small change in one of the parameters.

**Figure 10.** Ground state diagram for the $J_1 - J_2 - D_1 - D_2$ model with $|J_1| = 1$ and $D'_1 = 1$. The ground states and their energies are shown in table 17 and the equations of the coexistence lines are indicated in the table 18. We consider the dimensionless quantities $D'_1 = D_1/|J_1|$ and $J'_2 = J_2/|J_1|$.

**Table 17.** Spin configurations and ground states energies $J_1 - J_2 - D_1 - D_2$ model with $|J_1| = 1$ and $D'_1 = 1$ (corresponding to figure 10).

| $s'_1 s'_2$ | $s_1 s_2$ | $J_1$ | Energy | Region |
|------------|------------|-------|---------|--------|
| $\pm 2 \pm 1$ | $\mp 1 \mp 2$ | $J_1 > 0$ | $-8|J_1| - 4J_2 - 8D_1 - 2D_2$ | I |
| $\pm 2 \pm 1$ | $\mp 1 \mp 2$ | $J_1 < 0$ | | |
| $\pm 2 \pm 1$ | $\mp 1 \mp 2$ | $J_1 > 0$ | $-6|J_1| - 2J_2 - 5D_1 - 2D_2$ | II |
| $\pm 1 \pm 1$ | $\mp 1 \mp 1$ | $J_1 > 0$ | $-4|J_1| - J_2 - 2D_1 - 2D_2$ | III |
| $\pm 1 \pm 1$ | $\mp 1 \mp 1$ | $J_1 < 0$ | | |
| $0 \mp 1$ | $0 \mp 1$ | $J_1 > 0$ | $-2D_2$ | IV |
| $ \pm 1 \pm 0$ | $\mp 1 \mp 1$ | $J_1 < 0$ | | |
| $\pm 1 \pm 0$ | $\mp 1 \mp 1$ | $J_1 > 0$ | $-2|J_1| - D_1 - 2D_2$ | V |
| $\pm 1 \pm 0$ | $\mp 1 \mp 1$ | $J_1 < 0$ | | |
| $\pm 2 \pm 1$ | $\mp 1 \mp 1$ | $J_1 > 0$ | $-2|J_1| - 2J_2 - 5D_1 - 2D_2$ | VI |
| $\pm 2 \pm 1$ | $\mp 1 \mp 1$ | $J_1 < 0$ | | |
| $\pm 2 \pm 1$ | $\mp 1 \mp 1$ | $J_1 > 0$ | $-4|J_1| - 4D_1 - 2D_2$ | VII |
| $\pm 2 \pm 1$ | $\mp 1 \mp 1$ | $J_1 < 0$ | | |
| $\pm 2 \pm 1$ | $\mp 1 \mp 1$ | $J_1 > 0$ | $4J_2 - 8D_1 - 2D_2$ | VIII |

[119x88]the same energy. Notice that this diagram is considerably more complicated than the previous one, figure 9, because, as we already mentioned, $D'_1$ is a more relevant interaction that $D'_2$ since it affects the $S$ spins that can take more values. As in figure 5, there is a region of the parameter space where the ground state can change just by making a very small change in one of the parameters.
3.8. The $J_1 - J_3 - D$ model

Now in addition to $J_1$, we include $J_3$, the interaction between the $\sigma$ spins, next-nearest neighbors on the lattice, and study the case where the system feels an average crystal field $D$. The ground state phase diagram for this model is given in figure 11. The ground state configurations and their energies are shown in table 19, for the ferro
and the ferrimagnetic cases. The diagram has eight regions separated by four coexistence lines given in table 20. Notice that there is a large region of the phase diagram, region III, where the ground state has all the spins zero, this is due to the dominance of the large negative value of $-D$ that favors the spins zero. Likewise in the region of large positive values of $D$ the higher spins are favored.

### 3.9. The $J_1 - J_3 - D - h$ model

In this section we are going to show how the ground state diagram of the model described in the previous section, that includes interactions between the $S$ and $\sigma$ spins nearest neighbors on the lattice, the $\sigma$ spins next nearest neighbors on the lattice, and an average crystal field, changes when an external field $h$ is included. We study both cases: ferromagnetic and ferrimagnetic interactions between the $S$ and the $\sigma$ spins. We define the dimensionless quantities $\frac{1}{J_1} = \frac{h}{|J_1|}$ and $\frac{1}{J_3^2} = \frac{J_3}{|J_3|}$. We are doing this study with a fixed value of the crystal field.

#### 3.9.1. The $J_1 - J_3 - D - h$ model with ferrimagnetic ordering ($J_1 = -1, D = +1$)

Here we present the case where the interaction between the $S$ and $\sigma$ spins, nn on the lattice, is ferrimagnetic. The ground state diagram in the plane $J_3^2 = h'$ where $D' = 1$ and $J_1 = -1$ is presented in figure 12. The ground state configurations and their energies are shown in table 21. The diagram has six regions separated by eight
Depending on the parameter values the ground state can be ferro or ferrimagnetic. At the point $J' = -4$, $h' = 0$, four ground states coexist.

3.9.2. The $J_1 - J_2 - D - h$ model with ferromagnetic ordering ($J_1 = +1$, $D = +1$)

Now the interaction between the $S$ and $\sigma$ spins, nn on the lattice, is ferromagnetic. The ground state diagram in the plane $J' - h'$ where $D' = 1$ and $J_1 = +1$ is presented in figure 13. The ground state configurations and their energies are shown in table 23. The diagram has four regions separated by four coexisting lines given in table 24. Depending on the parameter values the ground state can be ferro or ferrimagnetic. At the point
In this work we have calculated the ground state phase diagrams of a mixed Ising model where spins $\sigma$ that can take three values $\pm 1$, 0, are located in alternating sites of a square lattice with spins $S$ that can take five values, $\pm 2$, $\pm 1$, 0. This model is relevant to the understanding of different molecular magnets that are currently been synthesized and that have many interesting magnetic properties. The Hamiltonian of the system has exchange interactions between nearest-neighbors, $S - \sigma$, between next nearest neighbors, $S - S$ and $\sigma - \sigma$, crystal field, and an external field. For simplicity we present the diagrams as two dimensional plots for several combinations of parameters in the Hamiltonian. Besides being useful to check the reliability of the different techniques used to study finite temperature phase diagrams, and to understand the low temperature behavior of the system, these diagrams can be a valuable tool to identify regions in which the model can present an interesting magnetic behavior. As expected the diagrams increase in complexity as the number of parameters in the Hamiltonian increases, in particular when the crystal fields are included. In many cases the ground states are highly degenerated. The diagrams have a symmetry under the change $h \rightarrow -h$, but not under $D \rightarrow -D$ (the crystal field interaction is independent of the sign of the spin, it only depends on its square value). Then, the more complicated diagrams are the ones where $D$ changes, particularly when $D$, changes because it affects the spins $S$ whose squares can take more values. Large negative values of $D$ favored the spin zero. In a future work we will explore the finite temperature behavior near the coexistence regions.

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