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► To cite this version:

G. Buendía, M. Novotny. Critical Behavior of a Mixed Ising Ferrimagnet. Journal de Physique IV Proceedings, 1997, 07 (C1), pp.C1-175-C1-176. 10.1051/jp4:1997163 . jpa-00255110

HAL Id: jpa-00255110

<https://hal.science/jpa-00255110>

Submitted on 1 Jan 1997

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Critical Behavior of a Mixed Ising Ferrimagnet

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Abstract. The critical behavior of a 2-D mixed ferrimagnetic spin2-spin1/2 Ising model has been studied with Monte Carlo and transfer-matrix techniques. This model is relevant for understanding bimetallic molecular ferrimagnetic materials. We calculate the finite temperature phase diagram putting special attention to the location and characterization of compensation points. We found that a compensation temperature appears when the interaction between the next-nearest neighbors spins 1/2 is included.

1. INTRODUCTION

Ferrimagnetic ordering seems to play a crucial role in the behavior of a numerous group of molecular materials that are currently being synthesized by several experimental groups [1]. The different temperature dependence of the sublattices magnetizations in a ferrimagnet raises the interesting possibility of the existence of compensation points: temperatures where the resultant magnetization vanishes before the critical temperature is reached. The behavior of the compensation point has important technological applications particularly in the field of thermomagnetic recording.

Mixed Ising systems provide simple but interesting models to study ferrimagnetism. Mean and effective field theories predict the existence of tricritical and compensation points in mixed Ising systems that include only nearest-neighbors and crystal field interactions [2]. However, recent results based in non-perturbative techniques such as Monte Carlo and numerical transfer-matrix indicate that these predictions are not reliable, and strongly suggest that the existence of compensation points is associated with second order interactions [3][4]. In this article we applied Monte Carlo and transfer-matrix numerical techniques to study a mixed Ising system in which spins $S (\pm 2, \pm 1, 0)$ are intercalated in a square lattice with spins $\sigma (\pm 1/2)$ - spin2-spin1/2 model -. In a previous work it was shown that if only nearest-neighbors interactions and the crystal field are included, this model has no compensation point and no evidence of a tricritical point (predicted by mean-field theories) [4]. In this article we are going to study the effect of second-order interactions in the finite temperature phase diagram particularly in the location of the compensation point.

2. THE MODEL

The Hamiltonian of our model is the following

$$H = -J_1 \sum_{\langle nn \rangle} S_i \sigma_j - J_2 \sum_{\langle nn \rangle} S_i^2 \sigma_j - J_3 \sum_{\langle nnn \rangle} S_i S_l - J_4 \sum_{\langle nnn \rangle} \sigma_j \sigma_k - h \sum_{i,j} (S_i + \sigma_j) + D \sum_i S_i^2 \quad (1)$$

where, J_1, J_2, J_3 and J_4 are the exchange interaction parameters, h is the external field, and D is the crystal field, all in energy units. In order to have an antiferromagnetic coupling between nearest neighbors J_1 is chosen to be negative. The exact ground state diagrams and the critical temperatures for the J_1 -D model (for which the only parameters in the Hamiltonian different from zero are J_1 and D) have been published elsewhere [4]. Mean-field theory predicts that the J_1 -D model where $S = \pm 1, 0$ and $\sigma = \pm 1/2$, - spin1-spin1/2 model - has a compensation point, but Monte Carlo and transfer matrix results for both, the spin2-spin1/2 and spin1-spin1/2 cases, show that there is no compensation point for the J_1 -D model. For the spin1-spin1/2 model it was shown that the compensation point appears only when the interaction J_4 is included [3]. We are interested to see if this is also the case for the spin2-spin1/2 model presented here.

3. NUMERICAL TECHNIQUES

3.1 The Monte Carlo (MC) method

Data were obtained for a 60x60 square lattice with 10^5 MC steps per site after discarding the first 10^3 steps per site. Configurations were generated by sequentially sweeping through the lattice and flipping the spins one at a time according with the heat-bath algorithm. The critical temperatures, T_{crit} , were calculated by locating the maximum value of the specific heat. The compensation points, T_{comp} , were located by finding the crossing point between the absolute values of the sublattice magnetizations such that,

$$|M_1(T_{comp})| = |M_2(T_{comp})|, \quad \text{sign}(M_1(T_{comp})) = -\text{sign}(M_2(T_{comp})) \quad \text{and} \quad T_{comp} < T_{crit} \quad (2)$$

3.2 Transfer-Matrix (TM) calculations

Traditional numerical TM calculations were performed. The lattice was wrapped on a torus of finite width and infinite extent, and periodic boundary conditions were imposed. By calculating the ratio of the largest and next-largest eigenvalues of the TM and using the scaling form for the correlation length we obtain the finite strip estimates for the T_{crit} . The T_{comp} was obtained by looking at the temperature below T_{crit} at which the magnetization operator (calculated using the two largest eigenvectors of the TM) is zero.

Fig.1: Critical and compensation temperature .vs. J_4 for $D=0$ and $D=1$.

Fig.2: Total magnetization (M) and absolute values of the sublattice magnetizations, $|M_1|$, $|M_2|$.vs. temperature

4. RESULTS AND CONCLUSIONS

We find an excellent agreement between MC and TM results. The results indicate that a compensation point can not be induced in this model by nearest-neighbor interactions (J_1 - J_2 -h-D), even when the second order interaction J_3 is included, we still do not find a compensation point. The compensation point appears when the J_4 interaction, between the σ spins, is added (J_1 - J_4 -D model). In Fig 1. we show T_{crit} and T_{comp} as funtions of J_4 for a couple of values of D . Notice that the compensation temperature does not exist until the J_4 interaction takes a minimum positive value. This minimum value of J_4 decreases with increasing values of D . The T_{crit} always increases with $J_4 > 0$, but once T_{comp} appears it remains independent of J_4 , this behavior is expected, increasing J_4 above the minimum have the effect of keeping the σ sublattice ordered at higher temperatures (increasing T_{crit}) but has no effect on the T_{comp} that has already been reached when the S sublattice (weakly dependent on J_4) magnetization was equal but of opposite sign to the σ sublattice magnetization. Fig 2. shows an example were the distinctive behavior of the magnetization at T_{crit} and T_{comp} can be observed. At T_{comp} the sublattice magnetizations cancel each other, whereas at T_{crit} both go to zero independently. The dependence of the compensation point with the longer range interactions has already be found experimentally [5].

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