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Magnetic response of mixed Ising ferrimagnets in the presence of external magnetic fields*

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Abstract

In this work we are going to present a numerical study based on the Monte Carlo method of mixed Ising ferrimagnet on a square lattice. We are particularly interested in studying the magnetic response of the system to an external field and the behavior of the compensation temperature. We found that there is a strong dependence of the compensation temperature with the field. We also notice the existence of metaestable states with very long lifetimes and compensation points at lower temperatures that the ones for the stable states.

Key words: Ferrimagnetic; Ising; Monte Carlo.

Respuesta magnética de los ferrimagnetos de Ising en presencia de campos magnéticos externos

Resumen

En este trabajo vamos a presentar un estudio numérico basado en el Método de Monte Carlo de un ferrimagneto mixto de Ising en una red cuadrada. Estamos particularmente interesados en estudiar la respuesta magnética del sistema a el campo externo y el comportamiento de la temperatura de compensación. Encontramos que existe una fuerte dependencia entre la temperatura de compensación y el campo. También encontramos que existen estados metaestables de vida media muy larga y con puntos de compensación a temperaturas mas bajas que las de los estados estables.

Palabras clave: Ferrimagnético; Ising; Monte Carlo.

Introduction

Ferrimagnetic ordering seems to play a crucial role in the stable, crystalline room-temperature magnets, that are currently being synthesized by several experimental groups in search for materials with technological applications (1, 2). In a ferrimagnet the different temperature dependence of the sublattices magnetization raises the possibility of the appearance of compensation temperatures: temperatures below the critical point where the total magnetization is zero (3). The temperature dependence of the compensation point has important applications in the field of thermomagnetic recording.

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Mixed Ising systems are good models to study ferrimagnetic ordering (4, 5). Recent results show that these systems can have compensation points when their Hamiltonian includes second order interactions (6, 7). In this work we are interested to study how the compensation temperature is affected when the system is under the effect of an external field.

The Mixed Ising Model

Our model consists of two interpenetrating square sublattices. One sublattice has spins that can take two values 1/2, the other sublattice have spins S that can take three values, 1,0.

The Hamiltonian of the model is given by,

$$H \quad J_1 \quad_{<nn>} {}_i S_j \quad J_4 \quad_{<nnn>} \iota \quad \kappa \quad D \quad_j S_j^2 \qquad [1]$$

$$h \quad_i \iota \quad_j S_j$$

where the J are the exchange interaction parameters, D is the crystal field and h is the external field, all in energy units. We select J_1=-1 such that the coupling between the nearest neighbors spins is antiferromagnetic.

Previous studies with Monte Carlo and transfer matrix techniques have shown that when the external field h is zero the above model has a compensation temperature (6, 7). In this work we are going to study the effect of the external field on the compensation temperature.

Monte Carlo Calculations

We use standard importance sampling techniques (8) to simulate the model described by equation 1 on square lattices of LxL sites, with L=40 and periodic boundary conditions. Data were generated with 50.000 Monte Carlo steps per site after discarding the first 5000 steps. The error bars were taken from the standard deviation of blocks of 500 sites. We define $=1/k_B T$ and take the Boltzmann's constant, k_B=1. Our program calculates the internal energy per site,

$$E \quad \frac{1}{L^2}\langle H\rangle \qquad [2]$$

the sublattice magnetizations per site, M_1 and M_2 defined as,

$$M_1 \quad \frac{2}{L_2}\left\langle \quad_j S_j \right\rangle ;\ M_2 \quad \frac{2}{L_2}\left\langle \quad_i \quad_i \right\rangle \qquad [3]$$

and the total magnetization per spin, $M \quad \frac{1}{2}(M_1 \quad M_2)$.

The averages are taken over all the configurations, the sums over j are over all the sites with S spins and the sums over i are over all the sites with spins. Each sum has $L^2/2$ terms.

The compensation point, T_{comp}, is defined as the point where the two sublattice magnetizations cancel each other such that the total magnetization is zero, i.e.,

$$\left|M_1 \ T_{comp}\right| \quad \left|M_2 \ T_{comp}\right| \qquad [4]$$

and

$$sign(M_1(T_{comp}) \quad sign(M_2(T_{comp}) \qquad [5]$$

Notice that at the compensation temperature the sublattice magnetizations are not zero, whereas at the critical temperature the total magnetization is zero and the sublattice magnetizations are also zero.

Results

The first thing that we notice is that, when a external field is included, the shape of the magnetization curves strongly depends on the initial configuration. In Figure 1 we show the magnetization curves that result from two different initial configura-

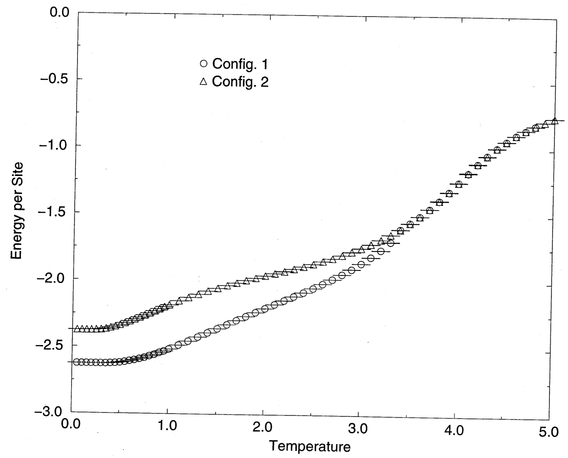

Figure 1. Total magnetization.vs. temperature for two different initial configurations, for D=0, J_4=6 and h=0.5. Config 1: S=1, =-1/2 (ground state); Config 2: S=-1, =+1/2.). At high temperatures both magnetization curves are the same. The compensation point is located at temperature where the total magnetization is zero

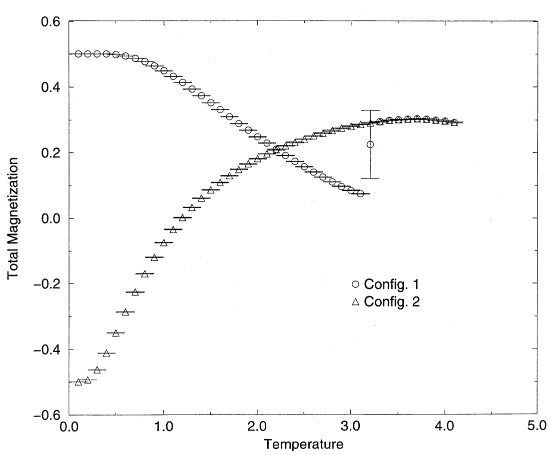

Figure 2. Total energy.vs. temperature for two different configurations, for D=0, J_4=6 and h=0.5. Config 1: S=1 =-1/2 (ground state); Config 2: S=-1 =+1/2.

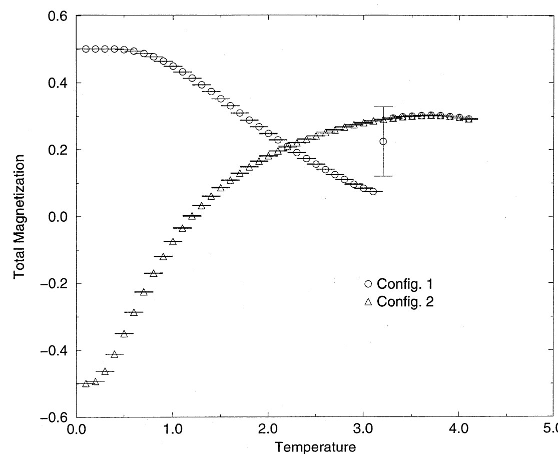

Figure 3. Total magnetization.vs. temperature for two different initial configurations, for D=0, J_4=6 and h=1. Config 1: S=1, =-1/2; Config 2: S=-1, =+1/2. Notice that the metaestable state, Conf:2, has a compensation point whereas the stable one has none.

tions, one of them the ground state (S=+1, =-1/2 for h=0.5). In Figure 2 we present the energy curves corresponding to Figure 1. It seems that, if we start with a configuration different from the ground state one, the system falls in a metaestable state with a lifetime much longer that our Monte Carlo run. The metaestable state evolves continuously to the stable state for high temperatures, however the state that started in the ground state configuration presents a discontinuity in the magnetization that seems to signal a first order phase transition. At low temperatures the antiferromagnetic interaction between nearest neighbors dominates, whereas at higher temperatures the system obeys the field, the transition between both regions happens at T_{crit}. We repeated this study for different values of h, and for lattices up to 200x200 sites and with much longer Monte Carlo runs and always get the same behavior: the discontinuity in the magnetization for the stable case and the ex-

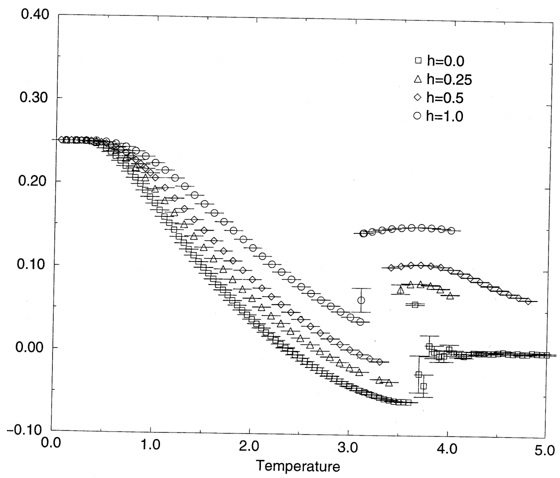

Figure 4. Behavior of the magnetization.vs. the temperature for different values of h,for D=0 and J_4=6. In all the cases the system started from the ground state configuration.

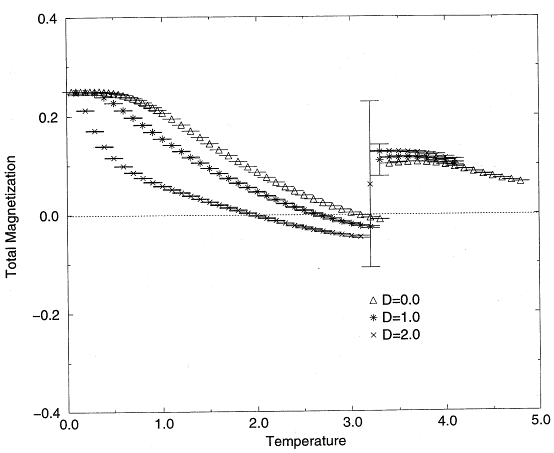

Figure 5. Total magnetization.vs. temperature for h=0.5, J_4=6 and different values of D.

istence of metaestable states with extremely long lifetimes.

It is important to remark that, in order to study the compensation temperature, we must be sure that we are in the stable regime. Notice that the metaestable case (Figure 1) seems to have a lower T_{comp} than the stable one. There are cases, at high h, where the metaestable state seems to have a compensation temperature where the stable state has none, Figure 3.

In Figure 4 we show the dependence of the total magnetization with the temperature for different values of the field (starting always from the ground state). Notice that the compensation temperature increases with the field until it disappear for a strong enough value of h. The crystal field has the opposite effect, it reduces the compensation temperature, see Figure 5. The minimum value of the external field at which the compensation temperature vanishes depends on the value of D.

Conclusions

There is a strong dependence of the compensation temperature with the external field and the crystal field. Since the compensation temperature is fundamental in several technological applications such as thermomagnetical recording, it is important to take in account that the external magnetic fields switch the value of the compensation temperature to higher values and that, for strong fields, there is no compensation temperature. The crystal field have the opposite effect.

We also notice that in the presence of external magnetic field this model has metaestable states with very long lifetimes and lower compensation temperatures than the stable ones.

Other interesting result of this work, that must be further investigated, is that the model seems to have a first order phase transition at high temperatures.

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