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Monte Carlo study of an anisotropic Ising multilayer with antiferromagnetic interlayer couplings

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HIGHLIGHTS

- Ferrimagnetic spin-1/2 Ising multilayer is studied.
- The system is composed of stacked non-equivalent planes with quenched site dilution in alternated planes.
- Interlayer couplings are antiferromagnetic.
- Monte Carlo simulations and the multiple histogram reweighting method are used to obtain the magnetic and thermodynamic properties of the system.
- Compensation phenomenon is found and compensation temperature is discussed.
- Phase diagrams are obtained.

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ABSTRACT

We present a Monte Carlo study of the magnetic properties of an Ising multilayer ferrimagnet. The system consists of two kinds of non-equivalent planes, one of which is site-diluted. All intralayer couplings are ferromagnetic. The different kinds of planes are stacked alternately and the interlayer couplings are antiferromagnetic. We perform the simulations using the Wolff algorithm and employ multiple histogram reweighting and finite-size scaling methods to analyze the data with special emphasis on the study of compensation phenomena. Compensation and critical temperatures of the system are obtained as functions of the Hamiltonian parameters and we present a detailed discussion about the contribution of each parameter to the presence or absence of the compensation effect. A comparison is presented between our results and those reported in the literature for the same model using the pair approximation. We also compare our results with those obtained through both the pair approximation and Monte Carlo simulations for the bilayer system.

1. Introduction

The study of ferrimagnetic materials has attracted considerable attention in the last few decades, especially since a number of phenomena associated with these materials present a great potential for technological applications [1–4]. In such systems the different temperature behavior of the sublattice magnetizations may cause the appearance of compensation points, i.e., temperatures below the critical point for which the total magnetization is zero while the individual sublattices remain magnetically ordered [5]. Although unrelated to critical phenomena, at the compensation point there are physical

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properties, such as the magnetic coercivity of the system, that exhibit a singular behavior [1,6,7]. The fact that the compensation point of some ferrimagnets occurs near room temperature makes them particularly important for applications in magneto-optical drives [1].

Initially, compensation effects were theoretically studied in bipartite lattices with different spin magnitudes in each sublattice [8,9]. However, this is not the only possible geometry which may lead to compensation phenomena. In particular, layered ferrimagnets have been extensively studied in the recent past [10–12]. In the latter case, systems are composed of stacked planes with different magnetic properties and the realization of antiferromagnetic couplings between adjacent layers has important technological applications such as in magneto-optical recordings [1], spintronics [2], the giant magnetoresistance [3], and the magnetocaloric effect [4]. In addition, the study of the magnetic properties of these systems is of great theoretical interest since it can provide insight into the crossover between the characteristic behavior of two- and three-dimensional magnets.

In recent experimental works, we find examples of realization and study of such bilayer [13], trilayer [14,15], and multilayer [16–20] systems. From the theoretical stance, a bilayer system with Ising spins and no dilution has been studied via transfer matrix (TM) [21,22], renormalization group (RG) [23–25], mean-field approximation (MFA) [23], and Monte Carlo (MC) simulations [23,26]. A similar system with both Ising and Heisenberg spins has been studied in the pair approximation (PA) both without dilution [27] and with dilution [10]. There is also a recent work considering an Ising bilayer with site dilution in an MC approach [12]. For the multilayer system, the PA has also been applied to the model with Ising and Heisenberg spins, both with no dilution [28] and with dilution [11].

If all layers have the same spin (e.g., spin-1/2) and we have an even number of layers, it is necessary that different layers have different number of spins in them for the existence of a compensation effect, as discussed in Refs. [10–12]. It is also necessary that the layers have asymmetric intralayer exchange integrals and that the layers with stronger exchange integrals have less atoms than their weak-exchange counterparts. That is easy to achieve with site dilution. However, to the best of our knowledge, no numerical simulation methods have yet been applied to multilayer systems with site dilution.

With that in mind, in this work we present a Monte Carlo study of the magnetic properties of a spin-1/2 Ising system composed of two kinds of non-equivalent planes, **A** and **B**, stacked alternately. All intralayer interactions are ferromagnetic while the interlayer interactions are antiferromagnetic. We also consider the presence of site dilution in one of the kinds of planes. The simulations are performed with the Wolff algorithm [29] and with the aid of a reweighting multiple histogram technique [30,31]. The model is presented in Section 2, the simulation and data analysis methods are discussed in Section 3, and the results are presented and discussed in Section 4.

2. Model and observables

The multilayer system we study consists of a simple cubic crystalline lattice such that non-equivalent monolayers (**A** and **B**) are stacked alternately (see Fig. 1). The **A** planes are composed exclusively of **A**-type atoms while the **B** planes have **B**-type atoms as well as non-magnetic impurities. The Hamiltonian describing our system is of the Ising type with spin 1/2 and can be written as

$$-\beta\mathcal{H} = \sum_{\langle i\in A, j\in A\rangle} K_{AA}s_is_j + \sum_{\langle i\in A, j\in B\rangle} K_{AB}s_is_j\epsilon_j + \sum_{\langle i\in B, j\in B\rangle} K_{BB}s_is_j\epsilon_i\epsilon_j, \tag{1}$$

where the sums run over nearest neighbors, $\beta \equiv (k_BT)^{-1}$, T is the temperature, k_B is the Boltzmann constant, the spin variables s_i assume the values ± 1, the occupation variables ϵ_i are uncorrelated quenched random variables which take on the values $\epsilon_i = 1$ with probability p (spin concentration) or $\epsilon_i = 0$ with probability $1-p$ (spin dilution). The couplings are $K_{AA} > 0$ 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 given by $J_{\gamma\delta} = \beta^{-1}K_{\gamma\delta}$, where $\gamma = A, B$ and $\delta = A, B$.

For the purpose of the numerical analysis to be discussed in Section 3, we define some observables to be measured in our simulation. Namely the dimensionless extensive energy is given by $E \equiv \mathcal{H}/J_{BB}$, and the magnetizations of **A**-type atoms and **B**-type atoms are, respectively

$$m_A = \frac{1}{N_A}\sum_{i\in A} s_i, \tag{2}$$

$$m_B = \frac{1}{N_B}\sum_{j\in B} s_j\epsilon_j, \tag{3}$$

where $N_A = L^3/2$ is the total numbers of **A**-type atoms in the system and $N_B = pL^3/2$ is the number of **B**-type atoms. The total magnetization of the system is

$$m_{\text{tot}} = \frac{1}{2}\left(m_A + pm_B\right). \tag{4}$$

We also define the magnetic susceptibilities

$$\chi_\gamma = N_\gamma K\overline{\left(\langle m_\gamma^2\rangle - \langle|m_\gamma|\rangle^2\right)}, \tag{5}$$