Physica B: Physics of Condensed Matter 529 (2017) 73–79

Contents lists available at ScienceDirect

Physica B: Physics of Condensed Matter

journal homepage: www.elsevier.com/locate/physb

Ferrimagnetism and compensation temperature in spin-1/2 Ising trilayers

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ARTICLE INFO

Keywords:
Ferrimagnetism
Ising trilayer
Compensation temperature
Critical temperature
Effective-field theory
Mean-field theory

ABSTRACT

The mean-field and effective-field approximations are applied in the study of magnetic and thermodynamic properties of a spin-1/2 Ising system containing three layers, each of which is composed exclusively of one out of two possible types of atoms, **A** or **B**. The **A-A** and **B-B** bonds are ferromagnetic while the **A-B** bonds are antiferromagnetic. The occurrence of a compensation phenomenon is verified and the compensation and critical temperatures are obtained as functions of the Hamiltonian parameters. We present phase diagrams dividing the parameter space in regions where the compensation phenomenon is present or absent and a detailed discussion about the influence of each parameter on the overall behavior of the system is made.

1. Introduction

The interest in studies on ferrimagnets has increased considerably in the last few decades, particularly due to a number of phenomena associated with these systems that present great potential for technological applications [1–4]. Since the discovery of ferrimagnetism in 1948 [5], several theoretical models have been proposed to explain their magnetic behavior [6,7]. Essentially, in these models the ferrimagnet is described as a combination of two or more magnetically coupled substructures, e. g., sublattices, layers, or subsets of atoms within the system. Each substructure may exhibit a different thermal behavior for its magnetization and the combination of these different behaviors may lead to the appearance of some interesting phenomena such as compensation points, i. e., temperatures below the critical point for which the total magnetization is zero while the individual substructures remain magnetically ordered [5].

Mixed-spin Ising systems are often used as models to study ferrimagnetism. The occurrence of compensation in such systems has been verified in two-dimensional systems with a number of combinations of different spins (e.g. $s = 1/2, 1, 3/2, 2, 5/2$) [8–22]. Some single-spin systems, such as layered magnets composed of stacked non-equivalent ferromagnetic planes, have also been effectively used to model ferrimagnets. A bilayer Ising system with spin-1/2 and no dilution has been studied via transfer matrix (TM) [23,24], renormalization group (RG) [25–27], mean-field approximation (MFA) [25], and Monte Carlo (MC) simulations [25,28]. Also the pair approximation (PA) has been applied to study similar systems such as Ising-Heisenberg bilayers [29] and multilayers [30] with spin-1/2 and no dilution. Although site dilution is a crucial ingredient for the existence of a compensation point in a single-spin system with even number of layers, even with in the diluted systems the compensation effect will be present only under very specific conditions, as has been verified through PA calculations for the Ising-Heisenberg bilayer [31] and multilayer [32] and through MC simulations for the Ising bilayer [33] and multilayer [34].

In contrast, for an odd number of layers, site dilution is no longer a necessary condition for the existence of compensation in a single-spin system. This was in fact confirmed in a very recent effective-field approximation (EFA) study of Ising trilayer nanostructures [35] for a few particular cases of Hamiltonian parameter values. In order to study the conditions under which compensation effects may occur, we propose a simple model, which is treatable by theoretical approximations and may also be considerably easier to be built in experimental studies, when compared to previous ferrimagnetic models. The system we introduce in this work does not require the presence of dilution, which is time- and memory-consuming in numerical simulations and may be difficult to control in experimental set-ups. More specifically, we study a three-layer Ising model with two types of atoms (**A** and **B**, say), such that each layer is composed of only one type of atom. Only two parameters are involved, the ratios between different interactions. These parameters are changed, in order to establish the conditions for the appearance of the compensation effect. We compare two different theoretical approximations, which are easy to implement in the studied model.

The paper is organized as follows: the theoretical model for the trilayer system is presented in Sec. 2, in which we present the Hamiltonian for the system in Sec. 2.1, the mean-field analysis of the Hamiltonian in Sec. 2.2, and the effective-field analysis in Sec. 2.3. The numerical

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https://doi.org/10.1016/j.physb.2017.10.036
Received 1 August 2017; Received in revised form 21 September 2017; Accepted 8 October 2017
Available online 31 October 2017

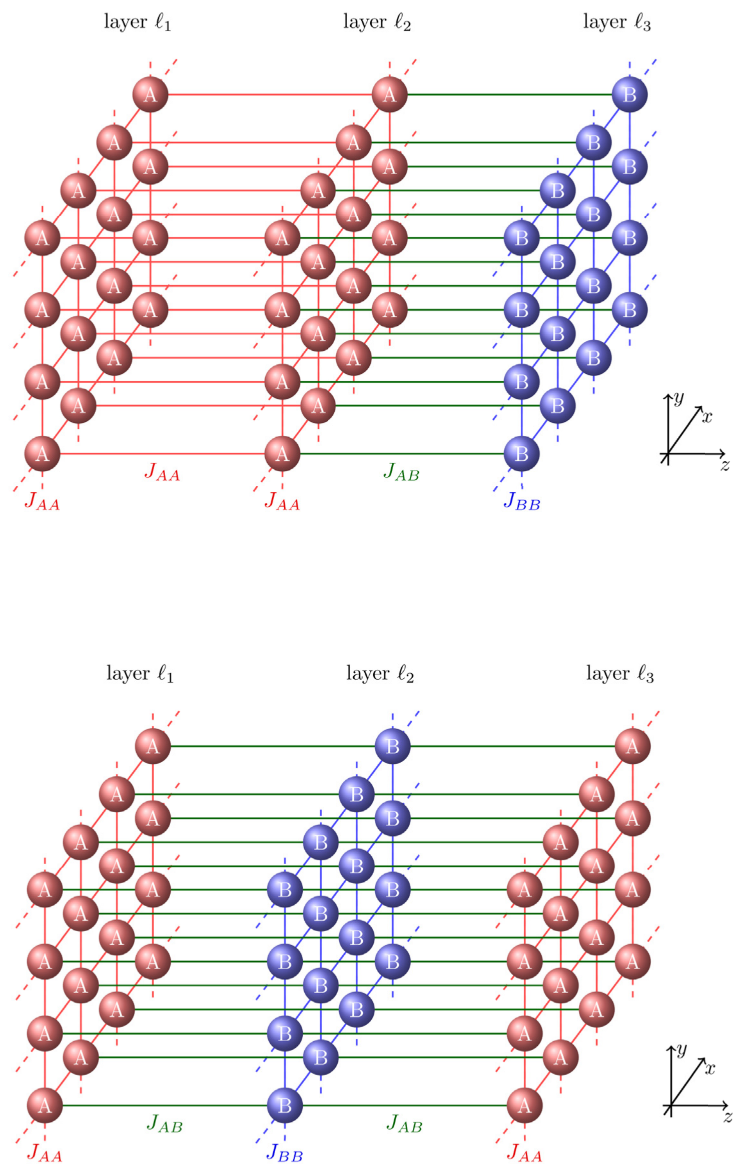

Fig. 1. A schematic representation of the trilayer systems. In (a), we have the **AAB** system, in which $J_{11} = J_{12} = J_{22} = J_{AA} > 0$, $J_{23} = J_{AB} < 0$, and $J_{33} = J_{BB} > 0$. In (b), we have the **ABA** system, in which $J_{11} = J_{33} = J_{AA} > 0$; $J_{12} = J_{23} = J_{AB} < 0$; $J_{22} = J_{BB} > 0$.

results are presented and discussed in Sec. 3 and our conclusion and final remarks in Sec. 4.

2. Theoretical model

2.1. Hamiltonian

The trilayer system we study consists of three monoatomic layers, ℓ_1, ℓ_2, and ℓ_3. Each layer is composed exclusively of either type-**A** or type-**B** atoms (see Fig. 1). The general system is described by the spin-1/2 Ising Hamiltonian

$$-\beta\mathcal{H} = \sum_{\langle i\in\ell_1, j\in\ell_1\rangle} K_{11} s_i s_j + \sum_{\langle i\in\ell_2, j\in\ell_2\rangle} K_{22} s_i s_j + \sum_{\langle i\in\ell_3, j\in\ell_3\rangle} K_{33} s_i s_j + \sum_{\langle i\in\ell_1, j\in\ell_2\rangle} K_{12} s_i s_j + \sum_{\langle i\in\ell_2, j\in\ell_3\rangle} K_{23} s_i s_j, \quad (1)$$

where the sums run over nearest neighbors, $\beta \equiv (k_B T)^{-1}$, T is the temperature, k_B is the Boltzmann constant, and the spin variables s_i assume the values ± 1. The couplings are $K_{\gamma\eta} \equiv \beta J_{\gamma\eta}$, where the exchange integrals $J_{\gamma\eta}$ are $J_{AA} > 0$ for **A-A** bonds, $J_{BB} > 0$ for **B-B** bonds, and $J_{AB} < 0$ for **A-B** bonds.

In this work we consider the two possible configurations of the trilayer with more atoms of type-**A** than type-**B** (see Fig. 1). The **AAB** system is the case in which $J_{11} = J_{12} = J_{22} = J_{AA}$, $J_{23} = J_{AB}$, and $J_{33} = J_{BB}$ (Fig. 1(a)), whereas the **ABA** system corresponds to $J_{11} = J_{33} = J_{AA}$, $J_{12} = J_{23} = J_{AB}$, and $J_{22} = J_{BB}$ (Fig. 1(b)). In both cases we wish to calculate the magnetization in each layer, $m_\gamma \equiv \langle s_{i\in\ell_\gamma}\rangle$, $\gamma = 1, 2, 3$, as well as the total magnetization

$$m_{\text{tot}} = \frac{1}{3}(m_1 + m_2 + m_3). \quad (2)$$