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Critical behavior of low dimensional magnetic systems

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ABSTRACT

In this study, critical behavior of low dimensional magnetic systems as cyano-bridged Tb(III)-Cr(III) bimetallic assembly was investigated with the mixed spin 3- spin 3/2 Ising model. The mixed spin Ising model is simulated with Cellular Automaton cooling and heating algorithms on one-dimensional lattices in periodic boundary conditions. The Ising model Hamiltonian includes only antiferromagnetic nearest-neighbor interaction ($J > 0$). The mixed spin system behaves like the isolated one-dimensional chain for zero magnetic field ($h = H/J = 0$). In the presence of the magnetic field, the magnetization is calculated using zero-field cooling (*ZFC*) and field cooling (*FC*) processes. The one-dimensional Ising model results are compatible with the cyano-bridged Tb(III)-Cr(III) bimetallic quasi-one dimensional assembly ($([Tb(H_2O)_2(DMF)_4\ \{Cr(CN)\}_6]\cdot H_2O$ (*DMF*=dimethylformamide)) results.

1. Introduction

Low dimensional magnetism has been a subject of studies for many years. In the last decades, new materials have been synthesized to obtain high temperature magnetism. One of these materials are cyano-bridged 4*f*–3*d* assemblies.*f*- block lanthanide ions having large anisotropic magnetic moments yield hard magnets and long-range magnetic order in solids [1–4]. Some of cyano-bridged 4*f*–3*d* assemblies also exhibit field-induced magnetic relaxation [3], cooling-rate dependent magnetism [5], photo-induced magnetization [6], and humidity response [7]. Interactions between the ions/molecules determine the electronic and magnetic properties as well as dimensionality of the assembly. Guo et al. synthesized cyano-bridged Tb (III) -Cr (III) bimetallic assembly ($[Tb(H_2O)_2(DMF)_4Cr(CN)_6]\cdot H_2O$ (*DMF*=dimethylformamide)) [1]. They introduced that antiferromagnetic interaction between Tb (III) and Cr (III) ions represented by S=3 and σ=3/2, respectively, leads to ferrimagnetic structure in the quasi-one dimensional zig-zag chain. A transition to 3D long-range magnetic order from the ferrimagnetic Tb (III) -Cr (III) chains occurs at T_C=5 K with the weak interchain interactions. Therefore, they draw attention to the requirement of the further experimental and theoretical studies to illuminate the magnetic interaction mechanism.

The aim of this study was to detect the interaction mechanism of the one-dimensional spin 3 - spin 3/2 chain. For this purpose, the one-dimensional spin 3 - spin 3/2 Ising model in its simplest form is simulated using Cellular Automaton (*CA*) and the results are compared with the experimental results to clear up the magnetic interaction mechanism. The one-dimensional Ising model was first introduced by Ernst Ising in 1925. The model established by Ising as a chain of spins, each spin interacts only with its nearest-neighbors, and an external field. At non-zero temperature, the model does not have any phase transition. Correlation lenght becomes infinite at H=T=0, which is the critical point of the model [8]. However, magnetic order can emerge with broken one-dimensionality due to orbital degeneracy or quasi-one dimensional geometry [1,9–14].

The mixed spin Ising model is a simple model to study ferrimagnetism. Therefore, a variety of spin mixtures, such as spin 1- spin 1/2 [15–22], spin 1 - spin 3/2 [23–25], spin 1 - spin 5/2 [26], spin 2 - spin 1/2 [15], spin 2 - spin 3/2 [27,28], spin 2 - spin 5/2 [29–34], spin 1/2 - spin 3/2 [15,21,35], spin 1/2 - spin 5/2 [15], spin 3/2 - spin 5/2 [17], and spin 3 - spin 3/2 [36] have been studied frequently by simulation and numerical methods. Creutz Cellular Automaton (*CCA*) algorithm and its improved versions are efficient to study the critical behaviors of the Ising model [36–40]. The *CCA* algorithm was first introduced by Creutz [41]. It is a microcanonical algorithm interpolating between the conventional Monte Carlo and the molecular dynamics techniques.

In this study, magnetization (M), susceptibility (χ), internal energy (U), and specific heat (C/k) are calculated on one-dimensional chain of linear dimension L=100, 500, 1000, 5000, 10,000, 50,000, and 100,000 with periodic boundary conditions. First, 1D behavior and the long-range order (*LRO*) of the mixed spin system have been investigated with temperature variation of the thermodynamic quantities in zero external field ($h = H/J = 0$) and external field ($h \neq 0$) using the Cellular Automaton cooling algorithm. At the same time, the thermodynamic quantities are calculated via field cooling (*FC*) and zero field cooling (*ZFC*) processes for $0 \leq h \leq 3.4$. For mixed spin systems,

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hysteresis curves are obtained at several temperature values. The blocking temperature (T_B) behavior and temperature dependence of the coercive field (H_C) were investigated by taking advantage of hysteresis curves. The outline of this paper is as follows: In Section 2, the model and the formalism are given. In Section 3, the results and the discussions are presented. A conclusion is given in Section 4.

2. Model

The mixed-spin Ising model hamiltonian is given by

$$H_I = J \sum_{<ij>} S_i \sigma_j - H \sum_i (S_i + \sigma_i) \tag{1}$$

where S_i=0, ± 1, ± 2, and ± 3 and σ_j= ± 1/2, ± 3/2. $\langle ij \rangle$ denotes the summation over all nearest -neighbor spin pairs in a one-dimensional lattice. J is the bilinear interaction ($J > 0$) between S and σ. H is the external field. The lattice is established from the two interpenetrating linear chains named as sublattice A and sublattice B. S and σ spins are located in sublattice A and sublattice B, respectively (Fig. 1). Three variables are associated with each site of the lattice. The values of these variables are determined in each site from its value and those of its nearest- neighbors at the previous time step. The updating rule, which defines a Cellular Automaton, is as follows: Of the three variables on each site, the first one is the Ising spin, A_i or B_j. Its values may be A_i=0, 1, 2, 3, 4, 5, and 6 for S and B_j=0, 1, 2, and 3 for σ. S and σ can be defined as S_i=(A_i-3) and σ_j=(2 B_j-3)/2 using the Ising spin variables in Eq. (1). The second variable corresponds the momentum variable which is conjugate to the spin (the demon). The kinetic energy associated with the demon, H_K, is an integer and it is equal to the change in the Ising spin energy (-dH_I) for any spin flip.

$$dH_I = H_I^t - H_I^{t+1} \tag{2}$$

Kinetic energy values lie in the interval (0, m) where m takes a different value for each h. For example, the greatest value of the dH_I equals −24 for J=1 and H=1. In those terms, m equals 48.

The total energy (TE) which is conserved is given in the following form:

$$TE = H_I + H_K \tag{3}$$

The third variable provides a checkerboard row style updating and so it allows the simulation of the Ising model on a cellular automaton. The black sites of the checkerboard are updated and then their color is changed into white; white sites are changed into black without being updated. The updating rules for the spin and the momentum variables are as follows: For a site to be updated its spin is changed to one of the other 6 (3) states with 1/6 (1/3) probability for S (σ) and the change in the Ising spin energy dH_I is calculated. If this energy change is transferable to or from the momentum variable associated with this site, such that the total energy TE is conserved, then this change is done and the momentum is appropriately changed. Otherwise, the spin and the momentum are not changed. For example, dH_I equals 24 in the case of σ_j^t=$-\frac{3}{2}$, $S_i^t = -3$, and $\sigma_{j+1}^t = -\frac{3}{2}$. S_i^{t+1} can take one of the S_i=3, 2, 1, 0, −1, −2, and −3 values at t+1 time step If the S_i^{t+1} takes the value of 3, the 24 unit energy is transferred to the system as the kinetic energy.

The system temperature for a given total energy is obtained from the average value of the kinetic energy, which is given by

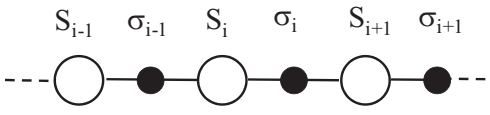

Fig. 1. One-dimensional lattice in periodic boundary conditions. Sublattice A and B generate the one-dimensional lattice. Sublattice A (B) is occupied by S (σ).

$$\langle E \rangle = \frac{\sum_{n=0}^{m} n e^{-nJ/kT}}{\sum_{n=0}^{m} e^{-nJ/kT}} \tag{4}$$

where E=H_K. The expectation value in Eq. (3) is average over the lattice and the number of time steps.

The field cooling (FC) process and the zero-field cooling (ZFC) process for Tb (III)-Cr (III) are carried out using the cooling and the heating algorithms of CA [36–40]. The cooling and the heating algorithms are divided into two basic parts, the initialization procedure and the taking of measurements. In the initialization procedure, firstly, all the spins in the lattice sites take ferrimagnetic ordered structure ($\uparrow(3), {}^{\downarrow}(-\frac{3}{2})$)) and the kinetic energy is given to a certain percentage of the lattice via the second variables in the black sites such that the kinetic energy of the site is equal to the change in the Ising spin energy for any spin flip. The values of the kinetic energy per site is set to obtain disordered spin configuration for zero field at high temperature. This configuration is run during the 20000 cellular automaton time steps. In the next step, the last configuration in the disordered structure at high temperature was chosen as a starting configuration for the FC and ZFC simulations. Rather than resetting the starting configuration at each energy, it was convenient to use the final configuration at a given energy as the starting point for the next.

2.1. FC *and* ZFC *processes*

In the measurement step of the FC algorithm, the last configuration of the initialization procedure in the disordered structure is taken as a starting configuration. The spin system is cooled for a value of non-zero field (h≠0). During the cooling cycle, a certain amount of energy per site are subtracted from the lattice through the second variable (H_K) after the 2000000 cellular automaton steps. In the zero-field cooling process (ZFC), the initial configuration in the disordered structure is used as a starting configuration for the cooling run at zero-field (h=0). The last configuration at low temperature of the cooling process is taken as a starting configuration for the heating run of the ZFC. Then the spin system is heated for a value of non-zero field (h≠0). During the heating cycle, a certain amount of energy per site is given to the lattice through the second variable (H_K) after the 2000000 cellular automaton steps. These energy amounts are determined considering the dH_I values for the possible spin configurations. Thus, the whole energy is used by the spin system. As a result, the spin system does not contain the remnant energy, which affects the temperature measurement.

3. Results and discussions

All simulations were carried out using the cooling and the heating algorithms improved from CCA for the one-dimensional spin 3 - spin 3/2 Ising model. The thermodynamic quantities (the order parameter (M), the susceptibility (χ), the internal energy (U), and the specific heat (C/k)) were computed over the lattice and over the number of time steps (2000000) after the discard of the first 100000 time steps during the development of the cellular automaton. Thus, the values of the thermodynamic quantities correspond to the equilibrium average values. The calculations were repeated by field cooling (FC) and the zero-field cooling (ZFC) processes on one-dimensional lattices with the linear dimensions L=100, 500, 1000, 5000, 10000, 50000, and 100000 for periodic boundary conditions.

The thermodynamic quantities are calculated from

$$M = \frac{1}{N} \sum_i S_i + \frac{1}{N} \sum_j \sigma_j \tag{5}$$

$$U = \frac{1}{H_0}((\sum_{<ij>} S_i \sigma_j) - h \sum_i (S_i + \sigma_j)) \tag{6}$$