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Monte Carlo investigation of the mixed spin Ising model with four-spin interaction and next-nearest neighbor couplings

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ABSTRACT

A Monte Carlo method is used to investigate the phase diagram of the ferromagnetic two-dimensional mixed spin-1 and spin-1/2 Ising model with four-spin interaction J_4 and next-nearest couplings J'. In the absence of this latter interaction, the system does not present any evidence for the tricritical point, whereas such behavior was suggested by finite cluster approximation. In the presence of the next-nearest neighbor interaction, the phase diagram is qualitatively and quantitatively different from that obtained with $J' = 0$. It undergoes two kinds of behaviors according to the negative and positive value of J'. In particular, for $J_4/J_2 = -4$ the system keeps the coexistence of the two ground states up to a J'-dependent finite temperature. In addition to the phase diagrams, the thermal dependence of the magnetizations have also been examined. Some characteristic features have been found which depend on the strengths of the interactions J_4 and J'.

1. Introduction

The Ising model continues to be one of the most frequently studied models in statistical mechanics, because of its simplicity and wide applicability. Recently, there has been considerable interest in experimental and theoretical researches of Ising model with multispin interactions. These models

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are interesting because they found their theoretical explanation in the theories of super exchange interaction, the magnetoelastic effect and the spin-phonon coupling [1]. Moreover, it was pointed out that the models with the higher-order exchange interactions may exhibit rich phase diagrams and can describe phase transition in some physical systems. Additionally, they show physical behavior not detected in the usual spin systems. For example, the deviation from $T^{3/2}$ Block law at low temperature [2] and the non universal critical phenomena [3,4]. For instance, the violation of universality is observed in the two-dimensional square lattice Ising model with nearest-neighbor, next-nearest neighbor, and four spin interactions [5,6].

From the theoretical point of view, the monoatomic Ising models with multispin interactions have been investigated in detail within different methods, such as mean field approximation [7,8], effective field theory [9,10], some more accurate treatments such as series expansion [11,12], renormalization group methods [13], Monte Carlo simulations [14], and also exact calculations [15,16]. Experimentally, an interesting fact for the models with multispin interactions has been reported. Indeed, it can be used to describe various physical systems such as classical fluid [17], solid ^{3}He [18], lipid bilayers [19], and rare gases [20]. Moreover for some materials it has been shown that the multispin interactions play a significant role; and they are comparable or even much important than the bilinear ones. The models with pair and quartet interaction have been applied successfully to study and explain the existence of first order phase transition in squaric acid crystal $H_2C_2O_4$ [21]. Such models have been also used to describe thermodynamical properties of hydrogen-bonded ferroelectric $PbHPO_4$, $PbDPO_4$ [22], some copolymers [23] and optical conductivity [24] observed in cuprate ladder $La_XCa_{14-X}Cu_{24}O_{41}$. On the other hand, some experimental studies on $La_6Ca_8Cu_{24}O_{41}$ [25,26] and $La_4Sr_{10}Cu_{24}O_{41}$ [27] reveal that they could be explained by the introduction of the four-spin interaction. It is worthy to note here that this later plays an important role in the two dimensional antiferromagnet La_2CuO_2 [28], the parent material of high-T_C superconductors.

The inclusion of further-neighbor interactions would allow for a better modeling of real magnetic systems [29] and of course of all other systems that can be mapped onto the Ising models such as models of microemulsions [30]. Concerning the Ising model with next-nearest neighbor interactions (NNN), it is of interest, not only because of the existing theoretical questions (universality), but also because experimental work [31] has shown that real pseudo-two-dimensional systems exist and the model (Ising model with NNN) may have physical significance. Thus, it can model interesting physical system as notably gases adsorbed on a crystalline surface, or on layered crystals. Indeed, adsorbed monolayers at 50% coverage are also good physical analogs of NNN Ising square lattice [32].

Intense interest has been directed to study the magnetic properties of two-sublattices mixed spin Ising system. They have less translational symmetry than their single spin counterparts, and are well adapted to study a certain type of ferrimagnetism [33]. Experimentally, it has been shown that the MnNi(EDTA)-$6H_2O$ complex [34] is a good example of a mixed system. The mixed Ising model consisting of spin-1/2 and spin-1 with only two-bilinear interaction has been studied by the renormalization group techniques [35,36], by high temperature series expansion [37], by free fermions approximation [38] and by finite cluster approximation [39]. The introduction of the next nearest neighbor (N.N.N.) coupling has been studied using numerical transfer matrix techniques [40] and Monte Carlo simulation [41]. Attention has been devoted to study the ground-state and the influence of the NNN on the transition temperature.

In a very recent work [42], one of us (N.B) has studied the thermodynamical properties of the mixed spin Ising model with four-spin interactions on square lattice, using finite cluster approximation (FCA). For instance, it has been shown that the phase diagram displays a second-order transition line which ends in a tricritical point which depends on the strength of the four-spin interaction.

The first purpose of this paper is to investigate the phase diagrams and the magnetic properties of the ferromagnetic mixed spin Ising model with four-spin interaction on square lattice using Monte Carlo simulation and; in particular, compare our phase diagram with that obtained very recently by the finite cluster approximation. The second goal of this work is to examine the effects of the next-nearest neighbor interactions (N.N.N.) on the obtained magnetic properties. Since the NNN and the four spin interactions have important effects on 2D Ising real systems, this makes the suggested model extremely interesting from theoretical and simulation viewpoints. Our system can be described by the following Hamiltonian: