Mixed spin Ising model with four-spin interactions and crystal field

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Abstract: A mixed spin Ising model consisting of spin-1/2 and spin-1 with four-spin interactions and crystal field anisotropy is studied by the use of the finite cluster approximation based on a single-site cluster theory. The state equations are derived for the square lattice. It has been shown that the phase diagram of the system depends on the strength of four-spin interaction and exhibits a variety of interesting features.

Keywords: mixed spin, four-spin interaction, uniform crystal field.

I. Introduction

For the last few decades, special attention has been given to the study of Ising models with multispin interactions both theoretically and experimentally. The origin of such interactions found its theoretical explanation in the theories of the superexchange interaction, the magnetoelastic effect, the perturbation expansion, and the spin-phonon coupling [1]. The increasing interest in investigating models with higher-order interactions arises from the fact that, on the one hand, they may exhibit rich phase diagrams and can describe phase transitions in some physical systems. On the other hand, they show physical behaviors, not observed in the usual spin systems. For instance, they display the nonuniversal critical phenomena [2, 3].

From the theoretical point of view, monoatomic Ising models with multispin interactions have been studied within different methods, such as mean field approximation[4,5], effective field theory [6-8], series expansions[9,10], renormalization group methods [11], Monte Carlo simulations [12] and exact calculations[13]. Experimentally, the models with multipsin interactions can be used to describe different physical systems such as classical fluids [14], solid^3 He [15], lipid bilayers [16], metamagnets [17] and rare gases [18]. Moreover, it has been shown that for certain materiels, these interactions play a significant role and they are comparable or much important than the bilinear ones. Indeed, the models with pair and quartet interactions have been used to study and explain the existence of first-order phase transition in squaric acid crystal ($H_2C_2O_4$) [19]. Such models have been also applied to describe thermodynamical properties of hydrogen-bonded ferroelectrics $PbHPo_4$ and $PbDPo_4$ [20], copolymers [21], and optical conductivity [22] observed in the cuprate ladder $La_xCa_{14-x}Cu_{24}O_{41}$. It is worthy to note here that the four spin interaction plays an important role in the two-dimensional antiferromagnet ($La_2Cu_2O_4$) [23], the parent materiel of high-Tc superconductors.

Another problem of growing interest is associated with the magnetic properties of two-sublattice mixed spin Ising systems. Their investigations are important, since they have less translational symmetry than their single counterparts, and they are well adopted to study a certain type of ferrimagnetism [24]. Experimentally, it has been shown that the MnNi(EDTA)-6H_2O complex is an example of a mixed spin system [25]. The mixed spin Ising model consisting of spin-1/2 and spin-1 with only two-bilinear interaction has been studied by the renormalization group technique [26], by high temperature series expansions [27], by free fermion approximation [28], by finite cluster approximation [29], and Monte Carlo simulation [30]. The influence of the crystal-field interaction on the phase transition has been also investigated using finite cluster approximation [31] and renormalization group method [32] both in two and three dimensions. Moreover, it has been shown [33] that the fluctuations of the crystal field interaction modify qualitatively and quantitatively the phase diagrams. The introduction of multispin interactions in such systems certainly modifies their magnetic properties. Thus, in order to clarify these effects some attentions have been devoted to the study of the mixed spin Ising models with quartet interactions. Some exacts results have been found for the honeycomb lattice [34] and doubly decorated planar lattices [35].

The first purpose of this paper is to investigate the phase diagram of the mixed spin-1/2 and spin-1 Ising model with two and four-spin interactions and uniform crystal field on the square lattice.. Such systems can be described by the following Hamiltonian:

$$H = -J_2 \sum_{(i,j)} \sigma_i S_j - J_4 \sum_{(i,j,k,l)} \sigma_i \sigma_k S_j S_l + D \sum_i S_i^2 \quad (1)$$

The underlying lattice is composed of two interpenetrating sublattices. One occupied by the spins with spin moment σ = ±1/2 and the other one is occupied by spins with spin moment S= 0, ±1. The first summation is carried out only over nearest-neighbour pair of spins. The second term represents the four-spin interaction, where the summation is over all alternate squares, shaded in Fig.1.The last term describes the uniform crystal field. To this end, we use the finite cluster approximation [36,37] within the framework of a single site cluster theory.
The outline of this paper is as follows: In section II, we describe the theoretical framework and calculate the state equations. In section III, we investigate and discuss the phase diagrams.

II. Theoretical framework

The theoretical framework that we adopt in the study of the mixed spin-1/2 and spin-1 Ising model with two and four-spin interaction and uniform crystal field described by the Hamiltonian (1) is the finite cluster approximation (FCA) [36,37] based on a single-site cluster theory. We have to mention that this method has been successfully applied to a number of interesting pure and disordered spin Ising systems [31,38-40]. It has also been used for transverse Ising models [41-43] and semi-infinite Ising systems [44-47]. In all their applications, it was shown that the FCA improve qualitatively and quantitatively the results obtained in the frame of the mean-field theory. In this approach, attention is focused on a cluster comprising first a single selected spin σ_0 (S_0) and its neighbour spins $\{\sigma_1,\sigma_2,S_1,S_2,S_3,S_4\}$ ($\{S_1,S_2, \sigma_1,\sigma_2, \sigma_3,\sigma_4\}$) with which it directly interacts (see Figures (b) and (c)).
We split the total Hamiltonian (1) into two parts, $H=H_0+H'$, where H_0 includes all parts of H associated with the lattice site 0. In the present system, H_0 takes the form

$$H_{0\sigma} = -\left[J_2 \sum_{i=1}^{4} S_i + J_4(S_1 S_2 \sigma_1 + S_3 S_4 \sigma_2)\right]\sigma_0 \quad (2)$$

$$H_{0S} = -\left[J_2 \sum_{j=1}^{4} \sigma_j + J_4(\sigma_1\sigma_2 S_1 + \sigma_3\sigma_4 S_2)\right]S_0 + DS_0^2 \quad (3)$$

Whether the lattice site 0 belongs to or S- sublattice, respectively.
The problem consists in evaluating the sublattice magnetizations and the quadrupolar moment. To this end, we denote by $\langle\sigma_0\rangle_c$ and $\langle S_0^n\rangle_c$ $(n = 1,2)$, respectively the mean value of σ_0 and S_0^n for a given configuration c of all other spins (i.e. when all other spin σ_i and S_j (i , j≠0) are kept fixed).
$\langle\sigma_0\rangle_c$ and $\langle S_0^n\rangle$ are given by

$$\langle\sigma_0\rangle_c = \frac{Tr_{\sigma_0}\, \sigma_0 \exp(-\beta H_{0\sigma})}{Tr_{\sigma_0} \exp(-\beta H_{0\sigma})} \quad (4)$$

$$\langle S_0^n\rangle_c = \frac{Tr_{S_0}\, S_0^n \exp(-\beta H_{0S})}{Tr_{S_0} \exp(-\beta H_{0S})} \quad (5)$$

Where $Tr_{\sigma 0}$ (or Tr_{S0}) means the trace performed over σ_0 (or S_0) only. As usual $\beta = 1/_T$ where T is the absolute temperature. The sublattice magnetizations, m and the quadrupolar moment q are then given by

$$\mu \equiv \langle\langle\sigma_0\rangle_c\rangle = \langle \frac{Tr_{\sigma_0}\, \sigma_0 \exp(-\beta H_{0\sigma})}{Tr_{\sigma_0} \exp(-\beta H_{0\sigma})} \rangle \quad (6)$$

$$m \equiv \langle\langle S_0\rangle_c\rangle = \langle \frac{Tr_{S_0}\, S_0 \exp(-\beta H_{0S})}{Tr_{S_0} \exp(-\beta H_{0S})} \rangle \quad (7)$$

$$q \equiv \langle\langle S_0^2\rangle_c\rangle = \langle \frac{Tr_{S_0}\, S_0^2 \exp(-\beta H_{0S})}{Tr_{S_0} \exp(-\beta H_{0S})} \rangle \quad (8)$$

Which can be considered as the starting point of the single site cluster approximation. <…> denotes the average over all spin configurations. Performing the inner traces in (6) ((7) and (8)) over the states of the selected spin σ_0 (S_0),we obtain

$$\mu = \langle \frac{1}{2} \tanh\left[\frac{K}{2}\{(S_1+S_2+S_3+S_4) + \alpha(S_1S_2\sigma_1 + S_3S_4\sigma_2)\}\right] \rangle \quad (9)$$

$$m = \langle \frac{2\sinh[K\{(\sigma_1+\sigma_2+\sigma_3+\sigma_4) + \alpha(\sigma_1\sigma_2S_1 + \sigma_3\sigma_4S_2)\}]}{\exp(\beta D) + 2\cosh[K\{(\sigma_1+\sigma+\sigma_3+\sigma_4) + \alpha(\sigma_1\sigma_2S_1 + \sigma_3\sigma_4S_2)\}]} \rangle \quad (10)$$

$$q = \langle \frac{2\cosh[K\{(\sigma_1+\sigma_2+\sigma_3+\sigma_4) + \alpha(\sigma_1\sigma_2S_1 + \sigma_3\sigma_4S_2)\}]}{\exp(\beta D) + 2\cosh[K\{(\sigma_1+\sigma_2+\sigma_3+\sigma_4) + \alpha(\sigma_1\sigma_2S_1 + \sigma_3\sigma_4S_2)\}]} \rangle \quad (11)$$

where $K = \beta J_2 \quad and \quad \alpha = \frac{J_4}{J_2}$

It is a formidable task to calculate the average on the right-hand side of Eqs.(9) to(11) over all spin

configurations. We can easily observe that any function such as $f(\sigma,S)$ of σ and S can be written as the linear superposition

$$f(\sigma,S) = f_1 + f_2\sigma + f_3 S + f_4 S^2 + f_5 \sigma S + f_6 \sigma S^2 \quad (12)$$

With appropriate coefficients f_i (i=1,…….,6). After applying this to all spins σ_i and S_j in expressions between brackets in Equations (9) to (11), we average over all spin configurations. In this paper we use the simplest approximation in which we treat all spin self-correlations exactly while still neglecting correlations between quantities pertaining to different sites. This leads to the following coupled equations

$$\mu = \mu\left[2\overline{A_1}q^2 + 4\overline{A_2}q^3 + 2\overline{A_3}q^4\right] + m\left[4\overline{A_4} + 4\overline{A_5}q + 8\overline{A_6}q + 4\overline{A_7}q^2 + 8\overline{A_8}q^2 + 4\overline{A_9}q^3\right] + m\mu^2\left[4\overline{A_{10}}q^3\right] + \mu m^2\left[2\overline{A_{11}} + 4\overline{A_{12}}q + 8\overline{A_{13}}q + 2\overline{A_{14}}q^2 + 8\overline{A_{15}}q^2 + 2\overline{A_{16}}q^2\right] + m^3\left[\overline{A_{17}} + \overline{A_{18}}q\right] + \mu m^4\left[2\overline{A_{19}}\right] + \mu^2 m^3\left[4\overline{A_{20}}q\right] \quad (13)$$

$$m = \mu\left[4\overline{B_1} + 8\overline{B_2}q + 4\overline{B_3}q^2\right] + m\left[2\overline{B_4} + 2\overline{B_5}q\right] + \mu^3\left[4\overline{B_6} + 8\overline{B_7}q + 4\overline{B_8}q^2\right] \quad \mu^2 m\left[2\overline{B_9} + 2\overline{B_{10}} + 8\overline{B_{11}} + 2\overline{B_{12}}q + 2\overline{B_{13}}q + 8\overline{B_{14}}q\right] + \mu m^2\left[4\overline{B_{15}}\right] + \mu^4 m\left[2\overline{B_{16}} + 2\overline{B_{17}}q\right] + \mu^3 m^2\left[4\overline{B_{18}}\right] \quad (14)$$

$$q = \left[\overline{D_1} + 2\overline{D_2}q + \overline{D_3}q^2\right] + \mu^2\left[6\overline{D_4} + 12\overline{D_5}q + 6\overline{D_6}q^2\right] + m^2\left[\overline{D_7}\right] + \mu m\left[4\overline{D_8} + 4\overline{D_9} + 4\overline{D_{10}}q + 4\overline{D_{11}}q\right] + \mu^4\left[\overline{D_{12}} + 2\overline{D_{13}}q + \overline{D_{14}}q^2\right] + \mu^3 m\left[4\overline{D_{15}} + 4\overline{D_{16}} + 4\overline{D_{17}}q + 4\overline{D_{18}}q\right] + \mu^2 m^2\left[6\overline{D_{19}}\right] + \mu^4 m^2\left[\overline{D_{20}}\right] \quad (15)$$

Where the coefficients are functions of K, α and D.
After some algebraic manipulations of Eqs. (13) to (15), we obtain an equation for of the form:

$$\mu = a\,\mu + b\mu^3 + \cdots \quad (16)$$

As usual the condition
a (K, α, D, d) =1 (17)
determines the second-order transition line.
The magnetization in the vicinity of the second order transition is given by

$$\mu^2 = \frac{1-a}{b} \quad (18)$$

The right hand side of (16) must be positive. If this is not the case, the transition is of the first order, and the point at which
a=1 and b=0 (19)
characterizes the tricritical point.

III. Results and discussions

Let us first investigate the phase diagram of the system, described by the Hamiltonian (1), in the absence of the crystal field (D=0). In this case, the system reduces to two sublattice mixed spin-1/2 and spin-1 Ising model with four-spin interaction. In Fig.2, we represent the variation of the critical temperature T_c with $\alpha = J_4/J_2$ by solving Eq.(19) as well as the tricritical condition (21) numerically. In this figure, the solid line represents the second-order transition which ends in a tricritical point (black point). This latter is found at

$$\left(\alpha_t = \frac{J_4}{J_2}\right)_t = 1.114\,;\ \left.\frac{T_c}{J_2}\right)_t = 1.196\ \right)$$

In the present work, we examine the effects of the four-spin interactions on the phase diagram of the mixed spin-1/2 and spin-1 Ising model with uniform longitudinal crystal field interaction, discussed previously by one of us (N.B) in [31]. In this case we have found (see Fig 2(a) for J_4=0) that the transition temperature decreases with increasing values of the crystal field D and ends in a tricritical point. The results of the influence of J_4 are summarized in Fig.2(a)-(b). These give the sections of the critical surface T_c (J_4,D) with planes of fixed values of the four-spin interaction less than α_c . In figure 2(a) we plot various transition lines when the system keeps its tricritical behaviour, namely in the range $-0.901 \leq$
$\leq$.
The T-component of the tricritical point decreases with the four-spin interaction and therefore there exists a tricritical line ending the second-order transition surface T_c (α,D). For the remaining range $-4 <$ $<$ -0.901 of the four spin interaction, the tricritical behavior disappears, and all transitions are always of second-order for any value of the crystal field D,as is plotted in figure.2(b). In particular, on the one hand an interesting behavior of the system can be seen in this figure when the four-spin interaction has an important negative value. Indeed, when α belongs to the range -4< α <-3.305, the system exhibits an "horizontal" re-entrance for relatively small values of the crystal field which becomes more important when α → -4. Thus, by increasing the value of D from D=0, the transition temperature T_c (α,D) increases and passes by a smooth maximum and then reduces rapidly to zero at the critical value D_c= $2J_2$ of the crystal field. We have to

note that the all second-transition lines vanish at that critical value D_c which is independent on the value of four-spin interaction

. -4< α <-0.901.On the other hand, we note the existence of a “vertical” re-entrance in a narrow range of the crystal field. This phenomena can be explained by a competition of energy E and entropy S in the free energy F=E-TS ; which is due in fact to the competition between pair interaction, quartet interaction and crystal field, when these latter take appropriate signs.

IV. Figures

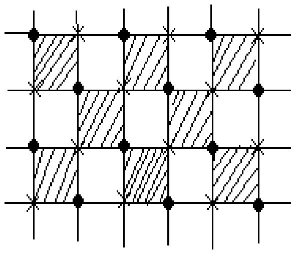
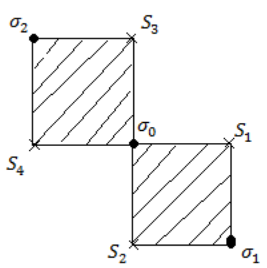


Fig.1.(a): Part of the square lattice. ● and ✕ correspond to and s sublattice sites, respectively.



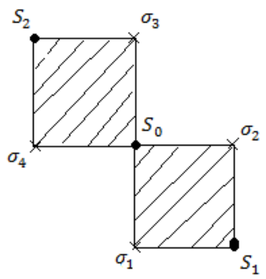


Fig.1. (b): Neighbours of spin with which it directly interacts.

Fig.1. (c): Neighbours of spin with which it directly interacts.

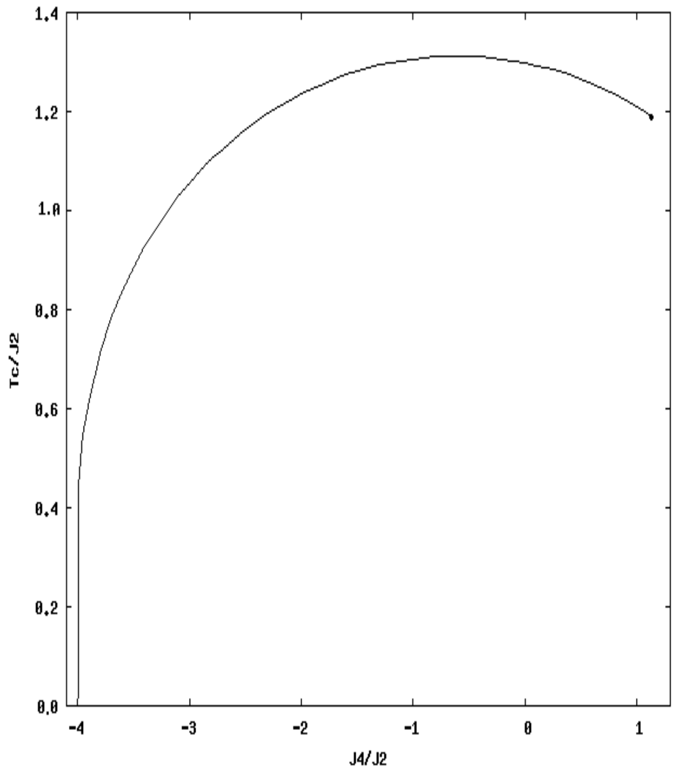


Fig.2: The phase diagram in (J_4/J_2, T_c/J_2) plane for the mixed spin-1/2 and spin-1 Ising model with four-spininteraction on a square lattice. The black point denotes the tricritical point.

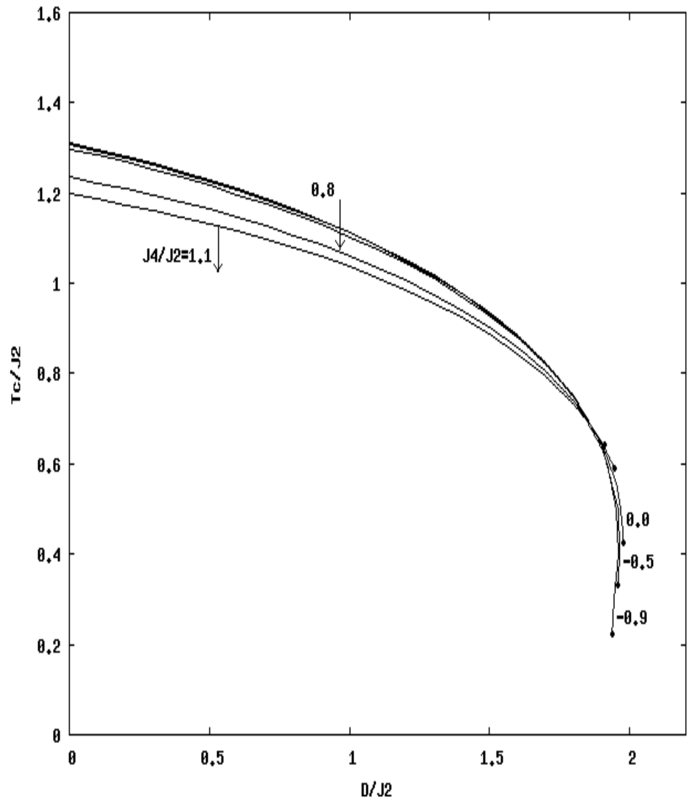


Fig.3. (a)

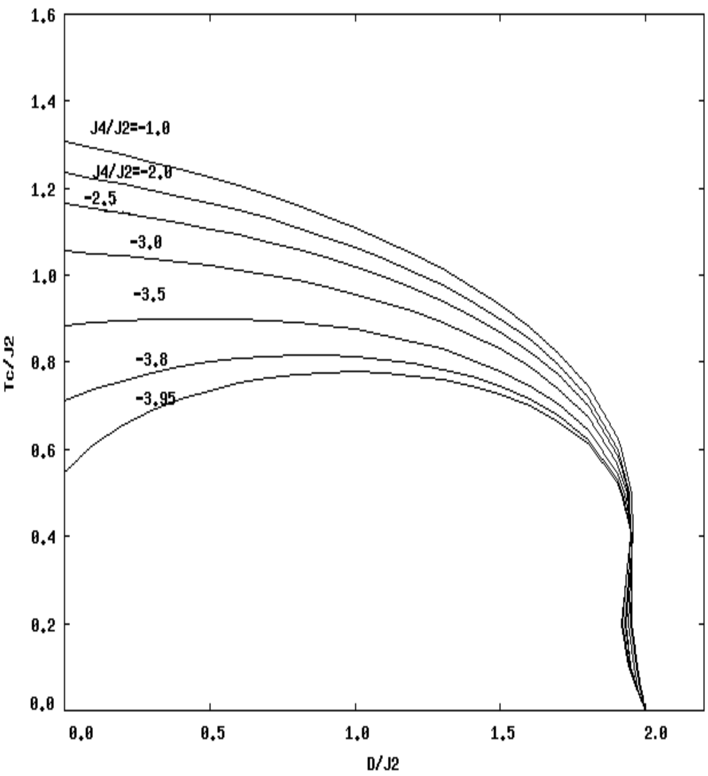


Fig.3. (b)

Fig.3: The phase diagrams in D-T plane .(a) when the system exhibits a tricritical behaviour ($-0.901J_2 < J_4 < 1.114 J_2$) .(b) when all transition lines are of second order ($-4J_2 < J_4 < -0.901J_2$) .The number accompanying each curve denotes the value of J_4/J_2. The black point denotes the tricritical point.

V. References

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