Phase diagram of the mixed spin transverse Ising model with four-spin Interactions

N.Benayad*, M.Ghliyem

Groupe de Mécanique Statistique, Laboratoire de physique théorique et appliquée, Faculté des sciences Aïn-Chock, Université Hassan II-Casablanca, B.P 5366 Maarif, Casablanca 20100, Morocco.

***Corresponding author: *E-mail: n.benayad@fsac.ac.ma ; noureddine_benayad@yahoo.fr Phone: + 212 5 22 23 06 84, Fax: + 212 5 22 23 06 74**

Abstract: The two dimensional mixed spin system consisting of spin-1/2 and spin-1 with four-spin interactions exhibits tricritical behaviour. The influence of a transverse field on this behaviour is studied with 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 system keeps its tricritical behaviour, but when the strength of the transverse field approaches a critical value, all transitions become of second-order for any value of four-spin interaction.

Keywords: mixed spin, four-spin interactions, transverse field.

I. Introduction

Over recent years, a particular interest has been devoted to the theoretical and experimental study of Ising models with multispin interactions. 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 behaviours not observed in the usual spin systems. For instance, they display a nonuniversal critical phenomena [1, 2].

Recently, the influence of multispin interactions and the crystal field on the mixed spin Ising models has been theoretically studied within different methods. Besides, finite cluster approximation [3], Monte Carlo simulation [4], and exact calculations [5]. Very recently, we have investigated [6], using the finite cluster approximation the influence of the fluctuation of the crystal field interaction on the mixed spin-1/2 and spin-1 Ising model with four-spin interaction.

The transverse Ising model was originally introduced by Blinc [7] and de Gennes [8] as a valuable model for the tunneling of the proton in hydrogen-bonded ferroelectrics [9] such as the KH_2PO_4 type. Since, then, it has been successfully applied to several physical systems, such as cooperative Jahn-teller systems [10] (like $DyVO_4$, and $TbVO_4$), ordering in rare earth compounds with a singlet crystal- field ground state [11] and also to some real magnetic materiels with strong uniaxial anisotropy in a transverse field [12].

From the theoretical point of view, monoatomic transverse Ising model with multispin interactions have been studied within the finite cluster approximation for the honeycomb and square lattice [13]. The mixed spin transverse Ising model [14] has been investigated by the finite cluster approximation [15], mean field renormalization group technique [16], and exact calculations [17, 18].

The purpose of this paper is to study the influence of the transverse field on the phase diagram of the mixed spin-1/2 and spin-1 Ising model with two and four-spin interactions on the square lattice. This system can be described by the following Hamiltonian:

$$H=-J_2\sum_{\langle ij\rangle}\sigma_{iz}S_{jz}-J_4\sum_{\{i,j,k,l\}}\sigma_{iz}\sigma_{kz}S_{jz}S_{lz}-\Omega\Big(\sum_i\sigma_{ix}+\sum_j S_{jx}\Big) \qquad (1)$$

where σ_α and S_α (α=x,z) are components of spin-1/2 and spin-1 operators.

The first summation is carried out only over nearest-neighbour pair of spins. The second term represents the four-spin interactions, where the summation is over all alternate squares, shaded in Fig.1. The last term describes the uniform transverse field. To this end, we use the finite cluster approximation [19,20] within the framework of a single-site cluster theory.

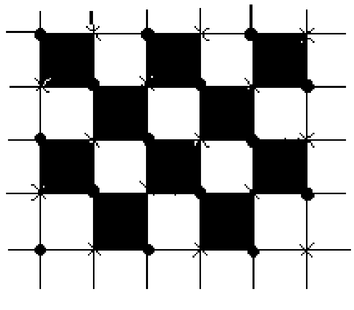


Fig .1: Part of the square lattice. ● and × correspond to σ and s-sublattice sites, respectively.

The outline of this work is as follows: In section 2, we give a description of the theoretical framework. In section 3, the phase diagrams of the system are investigated and discussed. We conclude this work in section 4.

I. Theoretical framework

The theoretical framework to be used in the study of the system described by the Hamiltonian (1) is the finite cluster approximation (FCA), based on a single-site cluster theory. In this approach, attention is focused on a cluster comprising just a single selected spin $\sigma_o(S_o)$ and its nearest 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 Fig .2(a,b)). We split the total Hamiltonian (1) into two parts, $H=H_o+H'$, where Ho includes all parts of H associated with the lattice site o. In the present system, H_o takes the form

$$H_{o\sigma}=A_1\sigma_{oz}+B_1\sigma_{ox} \tag{2}$$

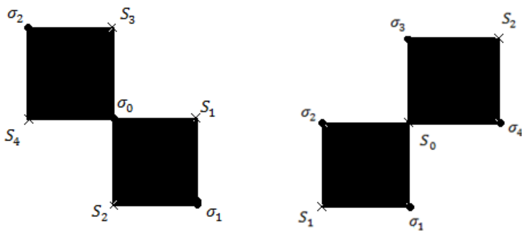
$$H_{os}=A_2S_{oz}+B_2S_{ox} \tag{3}$$

where

$$A_1=-J_2\sum_{j=1}^{4}S_{jz}-J_4\sum_{\{j,k,l\}}\sigma_{kz}S_{jz}S_{lz}\quad,\qquad B_1=-\Omega$$

$$A_2=-J_2\sum_{i=1}^{4}\sigma_{iz}-J_4\sum_{\{i,j,k\}}\sigma_{iz}\sigma_{kz}S_{jz}\quad,\qquad B_2=-\Omega \tag{4}$$

whether the lattice site o belongs to σ or S- sublattice, respectively.



(a) (b)

Fig.2: **(a)** Neighbours of spin σ_o with which it directly interacts.
(b) Neighbours of spin S_o with which it directly interacts.

First, the problem consists in evaluating the sublattice longitudinal and transverse components of the magnetizations and its quadrupolar moments. In order to calculate them, we choose a representation in which σ_{oz} and S_{oz} are diagonal and denote by $<\sigma_{o\alpha}>_c$ ($<(S_{o\alpha})^n>_c$, n=1,2) the mean value of $\sigma_{o\alpha}$ ($(S_{o\alpha})^n$) 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). Neglecting the fact that H_o and H' do not commute,
$<\sigma_{o\alpha}>_c$ and $<(S_{o\alpha})^n>_c$ are given by:

$$\left\langle\sigma_{o\alpha}\right\rangle_c=\frac{\mathop{\mathrm{Tr}}\limits_{\sigma_o}\sigma_{o\alpha}\exp(-\beta H_{o\sigma})}{\mathop{\mathrm{Tr}}\limits_{\sigma_o}\exp(-\beta H_{o\sigma})} \tag{5}$$

and

$$\left\langle S_{o\alpha}\right\rangle_c=\frac{\mathop{\mathrm{Tr}}\limits_{S_o}S^n_{o\alpha}\exp(-\beta H_{os})}{\mathop{\mathrm{Tr}}\limits_{S_o}\exp(-\beta H_{os})} \tag{6}$$

where $Tr_{\sigma o}$ (or Tr_{so}) means the trace performed over σ_o (or S_o) only. As usual ß=1/T where T is the absolute temperature. Therefore, the magnetizations μ_α, m_α (α=x,z) and the quadrupolar moment q_α are given by

$$\mu_\alpha\equiv\left\langle\left\langle\sigma_{o\alpha}\right\rangle_c\right\rangle=\left\langle\frac{\mathop{\mathrm{Tr}}\limits_{\sigma_o}\sigma_{o\alpha}\exp(-\beta H_{o\sigma})}{\mathop{\mathrm{Tr}}\limits_{\sigma_o}\exp(-\beta H_{o\sigma})}\right\rangle, \tag{7}$$

$$m_\alpha\equiv\left\langle\left\langle S_{o\alpha}\right\rangle_c\right\rangle=\left\langle\frac{\mathop{\mathrm{Tr}}\limits_{S_o}S_{o\alpha}\exp(-\beta H_{os})}{\mathop{\mathrm{Tr}}\limits_{S_o}\exp(-\beta H_{os})}\right\rangle, \tag{8}$$

and

$$q_\alpha\equiv\left\langle\left\langle S^2_{o\alpha}\right\rangle_c\right\rangle=\left\langle\frac{\mathop{\mathrm{Tr}}\limits_{S_o}S^2_{o\alpha}\exp(-\beta H_{os})}{\mathop{\mathrm{Tr}}\limits_{S_o}\exp(-\beta H_{os})}\right\rangle, \tag{9}$$

which can be considered as the starting point of the single-site cluster approximation. <……> denotes the average over all spin configurations. Eqs (7) to (9) are not exact. Nevertheless they have been accepted as a reasonable starting point [21] for transverse ising systems and have been successfully applied to a number of interesting transverse Ising systems [22,23-25].We have to emphasize that the Ising limit (Ω=0),Hamiltonian (1) contains only σ_{iz} and S_{jz}.Then, relations(7)-(9) become exact identities. To calculate $<\sigma_{o\alpha}>_c$ and $<(S_{o\alpha})^n>_c$ one has first to diagonalize the single site Hamiltonians $H_{o\sigma}$ and H_{os} , respectively. To do this, it is convenient to use the following rotation transformations:

$$\sigma_{oz}=\cos\varphi\sigma'_{oz}-\sin\varphi\sigma'_{ox} \tag{10}$$

$$\sigma_{ox}=\sin\varphi\sigma'_{oz}+\cos\varphi\sigma'_{ox} \tag{11}$$

$$S_{oz}=\cos\phi S'_{oz}-\sin\phi S'_{ox} \tag{12}$$

$$S_{ox}=\sin\phi S'_{oz}+\cos\phi S'_{ox} \tag{13}$$

where
$$\cos\varphi=\frac{-A_1}{\sqrt{A_1^2+B_1^2}}\qquad\sin\varphi=\frac{-B_1}{\sqrt{A_1^2+B_1^2}} \tag{14}$$

$$\cos\phi=\frac{-A_2}{\sqrt{A_2^2+B_2^2}}\qquad\sin\phi=\frac{-B_2}{\sqrt{A_2^2+B_2^2}} \tag{15}$$

The coordinate rotations (10) to (13) turn the Hamiltonians $H_{o\sigma}$ and H_{os} into diagonal forms. Then, evaluating the inner traces in (7) to (9) over the states of the selected spins σo(So), we obtain:

$$\mu_z=\left\langle\frac{-A_1}{2\sqrt{A_1^2+B_1^2}}\tanh\left[\frac{\beta}{2}\sqrt{A_1^2+B_1^2}\right]\right\rangle \tag{16}$$

$$m_z=\left\langle\frac{-A_2}{\sqrt{A_2^2+B_2^2}}\frac{2\sinh\left(\beta\sqrt{A_2^2+B_2^2}\right)}{1+2\cosh\left(\beta\sqrt{A_2^2+B_2^2}\right)}\right\rangle \tag{17}$$

$$q_z = \left\langle \frac{-A_2}{\sqrt{A_2^2+B_2^2}} \frac{2\sinh\left(\beta\sqrt{A_2^2+B_2^2}\right)}{1+2\cosh\left(\beta\sqrt{A_2^2+B_2^2}\right)} \right\rangle \quad (18)$$

It is a formidable task to calculate the average on the right-hand side of Eqs.(16) to (18) 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

$$f(\sigma,S) = f_1 + f_2\sigma + f_3 S + f_4 S^2 + f_5\sigma S + f_6\sigma S^2 \quad (19)$$

with appropriate coefficients f_i (i=1,….,6) . After applying this to all spins σ_i and S_j in expressions between brackets in Eqs. (16) to (18), 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:

$$\begin{aligned}\mu_z =\ & \mu_z[2A_1 q_z^2 + 4A_2 q_z^3 + 2A_3 q_z^4] + m_z[4A_4 + 4A_5 q_z \\ & + 4A_6 q_z^2 + 4A_7 q_z^3] + m_z\mu_z^2[4A_8 q_z^3] + \\ & \mu_z m_z^2[2A_9 + 4A_{10}q_z + 2A_{11}q_z^2] + m_z^3[4A_{12} + \\ & 4A_{13}q_z] + \mu_z m_z^4[2A_{14}] + \mu_z^2 m_z^3[4A_{15}q_z]\end{aligned} \quad (20)$$

$$\begin{aligned}m_z =\ & \mu_z[4B_1 + 8B_2 q_z + 4B_3 q_z^2] + m_z[2B_4 + 2B_5 q_z] + \\ & \mu_z^3[4B_6 + 8B_7 q_z + 4B_8 q_z^2] + \mu_z^2 m_z[2B_9 + 2B_{10}q_z] \\ & + \mu_z m_z^2[4B_{11}] + \mu_z^4 m_z[2B_{12} + 2B_{13}q_z] + \mu_z^3 m_z^2[4B_{14}]\end{aligned} \quad (21)$$

$$\begin{aligned}q_z =\ & [C_1 + 2C_2 q_z + C_3 q_z^2] + \mu_z^2[6C_4 + 12C_5 q_z + 6C_6 q_z^2] \\ & + m_z^2[C_7] + \mu_z m_z[4C_8 + 4C_9 q_z] + \mu_z^4[C_{10} + 2C_{11}q_z \\ & + C_{12}q_z^2] + m_z\mu_z^3[4C_{13} + 4C_{14}q_z] + \mu_z^2 m_z^2[6C_{15}] + \\ & m_z^2\mu_z^4[C_{16}]\end{aligned} \quad (22)$$

where the coefficients are functions of K, α, and Ω.
After some algebraic manipulations of Eqs (20) to (22), we obtain an equation for μ_z of the form

$$\mu_z = a\,\mu_z + b\,\mu_z^3 + \ldots\ldots \quad (23)$$

As usual the condition

$$a(K, \alpha, \Omega)=1 \quad (24)$$

determines the second-order transition line. The magnetization μ_z in the vicinity of the second-order transition is given by

$$\mu_z^2 = \frac{1-a}{b} \quad (25)$$

The right hand side of (25) must be positive. If this is not the case, the transition is of the first-order, and the point at which

$$a(K,\alpha,\Omega)=1 \quad \text{and} \quad b(K,\alpha,\Omega)=0 \quad (26)$$

characterizes the tricritical point.

II.Results and discussion

In this section, we illustrate some results for the system under investigation. Indeed, we study the effect of the transverse field Ω, as well as the four-spin interactions J_4 on the phase diagram of the mixed spin Ising model.
First of all, we determine the phase diagram of the mixed spin transverse Ising system in the absence of the four-spin interactions (i.e.$\alpha=J_4/J_2=0$). As clearly seen in figure 3, the critical temperature decreases from its maximum value in the mixed Ising model $T_c(\Omega=0)$ to vanish at a critical value $\Omega_c/J_2=2.117$.

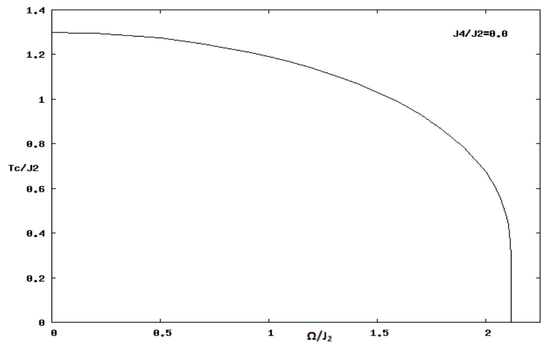


Fig.3: The phase diagram in T-Ω plane of the mixed spin-1/2 and spin-1 transverse Ising model on the square lattice when $J_4/J_2=0$.

In order to have an idea on the effects of the transverse field Ω on the mixed spin Ising model with four-spin interactions, we have plotted in figure4, the phase diagram in the (T/J_2,J_4/J_2) plane, for selected values of the transverse field. When this latter belongs to the range $0\leq\Omega_c/J_2\leq1.826$ the critical temperature T_c increases with increasing values of J_4 and passes by a smooth maximum and then reduces to a tricritical point. The remaining part of the phase diagram ($1.826<\Omega_c/J_2\leq2.117$) shows a qualitatively different behaviour from the previous range of Ω. Thus, the tricritical behaviour disappears and all transitions are always of second-order. We have to mention that the transverse field reduces the longitudinal ferromagnetic order and therefore acts against the order.

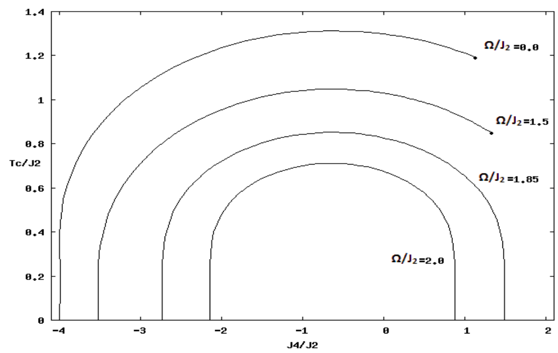
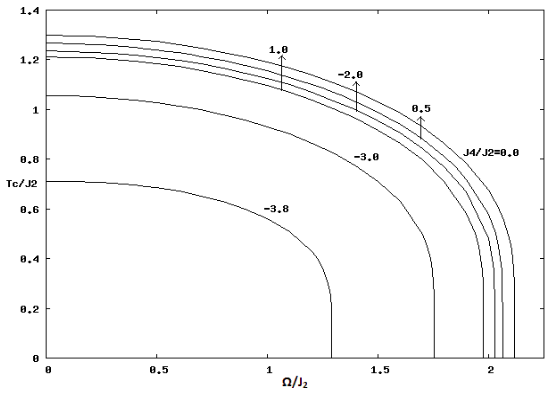
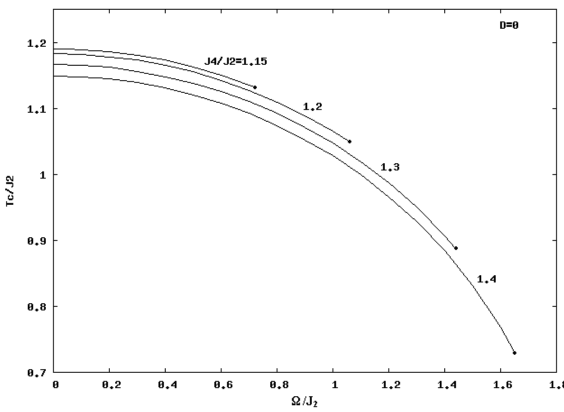


Fig.4: The phase diagram in T-J_4 plane. The number accompanying each curve denotes the value of Ω/J_2. The black point denotes the tricritical point.

In figure 5, we plot various transition lines in the (T/J_2, Ω/J_2) plane for fixed values of the J_4/J_2. So, the figure illustrates the influence of the four-spin interaction on the phase diagram of the mixed spin transverse Ising model. It shows that, for any given value of J_4/J_2 the critical temperature line starts from its J_4/J_2 dependent value at $\Omega=0$ and decreases gradually with increasing values of the transverse field. In this case, we note that the system exhibits second-order transition for large range of J_4/J_2 but in a narrow range of the four-spin interaction, the critical lines end in a tricritical point as is shown in Fig.5.b. We also notice that the Ω-component of the tricritical point increases with increasing the strength of the four-spin interaction.



(a)



(b)

Fig.5: The phase diagram in T- Ω plane, when all transition lines are of second order. The number accompanying each curve denotes the value of J_4/J_2. The black point denotes the tricritical point.

III.Conclusion

In this work, we have studied the mixed spin transverse Ising model, consisting of spin-1/2 and spin-1, with two and four-spin interactions J_4 on the square lattice. We have used the finite cluster approximation within the framework of a single-site cluster theory. In this approach we derived the state equations and investigated the phase diagram. This latter reveals that the system undergoes a second-order transitions and exhibits tricritical behaviour in certain ranges of the transverse field Ω.

.

References

[1] F.Y.Wu, Phys.Rev.B 4(1971)2312.
[2] L. P. Kadanoff, F. J. Wegner, Phys. Rev. B 4 (1971) 3989.
[3] M.Ghliyem and N. Benayad, M. J. cond. Matter 12 (2010) 244.
[4] A. Zaim, M.Kerouad, Y.Belmamoun, Physica B 404 (2009) 2280.
[5] S. Lacková, M. Jaščur, Czechoslovak journal of physics 51 (2001).
S. Lacková, M. Jaščur, Phys. Rev E 64(2001) 036126.
[6] N.Benayad, M. Ghliyem, Physica B (2011) in press.
[7] R. Blinc, J. Phys.Chem. Solids 13(1960)204.
[8] P.G. de Gennes, Solid State Commun.1(1963)132.
[9] R. Blinc , B. Zeks, Soft Modes in Ferroelectrics and Antiferroelectrics(North-Holland, Amsterdam,1974).
[10] R. J. Elliott, G. A. Gekring, A. P. Malozemoff, S. R. P. Smith, N. S. Staude, R. N. Tyte, J. Phys.C 4(1971)179.
[11] Y.L. Wang, B.Cooper, Phys. Rev 172(1968) 539.
[12] R. B. Stinchcombe,J.Phys.C 6(1973)2459.
[13] B. Laaboudi, M. Kerouad, Physica A 250 (1998)384.
[14] T.Kaneyoshi, Physica A 272 (1999) 545.
[15] N. Benayad, A. Fathi, L. Khaya, J. Magn. Magn. Mater 278 (2004) 407.
[16] N. Benayad, R. Zerhouni, A. Klümper, J.Zittartz, Physica A 262(1999) 483.
[17] Y.Q.Ma, Y.G. Ma, Phys lett A 173(2002)377.
[18] M. Jaščur, S.Lacková, J. Phys: Condens. Matter 12(2000) L 583.
[19] N. Boccara, Phys. lett. A 94 (1983) 185.
[20] A. Benyoussef, N. Boccara, J. Phys 44 (1983) 1143.
[21] F.C.Sá Barreto, I.P.Fittipaldi and B. Zeks, Ferroelectrics 39(1981)1103.
[22] N. Benayad, R. Zerhouni, Phys. Stat. Sol(b) 201(1997)491.
[23] N. Benayad, R. Zerhouni, A. Klümper, Eur. Phys. J. B 5 (1998) 687.
[24] N. Benayad, A. Fathi, R. Zerhouni, J. Magn. Magn. Mater 222 (2000) 355.
[25] F.C.Sá Barreto, I. P. Fattipaldi, Physica A 129(1985)360.