# NUMERCAL STUDY OF A FOUR COMPONENTS SYSTEM

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We have investigated numerically a statistical model of four component systems, which exhibit two critical temperatures, called the Ashkin-Teller model (ATM). The effects of, the anisotropy coupling, the single ion potential field and the mixed spin on the structure of the phase diagram have been studied. The model presents a rich variety of phase transitions which meet on tricritical or multicritical points. Different partially ordered phases with a partially broken symmetry appears at high temperatures. Their region of stability and their structure depend on the phase parameter space. The nature of critical lines which bound these partially ordered phases depends on the coupling parameters and the cristalline anisotripy".

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## I. INTRODUCTION

Ashkin and Teller (1943) have introduced a lattice statistical model, now known as the Ashkin-Teller model (ATM), in order to explain the two critical temperatures occurring in a four component systems [1]. For those systems, each site of the lattice is occupied by one of the four different types of atoms A, B, C or D. In terms of spin variables, it can be considered as a two superposed spin-½ Ising models which are described by variables $\sigma_i$ and $S_i$ sitting on each of the sites on an hypercubic lattice [2]. Within each Ising model, there is a two spin nearest-neighbour interaction $K_2$ and the different Ising models are coupled by a four spins interaction $K_4$. A good physical realisation for this model is the compound of Selenium adsorbed on Ni surface [3]. The Hamiltonian describing the ATM is given by:

$$H = -K_2 \sum_{<i,j>} (\sigma_i\sigma_j + S_iS_j) - K_4 \sum_{<i,j>} \sigma_i\sigma_j S_i S_j \qquad (1)$$

Where <ij> denotes a pair of nearest-neighbour spins of an hypercubic lattice.

This model has a rich structure in two dimensions. Using, in one hand connections with the 8-vertex model [4] and in the other hand the exact duality and symmetry considerations [5], some exact results are known. It was shown that the phase diagram of the ferromagnetic ATM presents three different phases [6,7,8]: Paramagnetic phase (P) (Completely symmetrical; where the thermal averages $<\sigma>=<S>=<\sigma S>=0$; Partially ordered phase (PO) (partial symmetry; $<\sigma>=<S>=0$ and $<\sigma S>\neq 0$) and the Baxter phase (Completely broken symmetry; $<\sigma>\neq 0$, $<S>\neq 0$ and $<\sigma S>\neq 0$). The Baxter-PO and PO-P critical lines describe Ising-like phase transitions and are related to each other by duality. The Baxter-P critical line is known exactly. It is the only self dual line whose along the exponents are varying continuously as it was confirmed by Monte Carlo (MC) simulations using the cluster algorithm [9]. The three critical lines meet at the four-state Potts ferromagnetic critical point. Since the critical lines are not all known exactly, different methods have been applied in order to study the structure of the phase diagram. Apart from the mean field approach (MFA) [10] which gives tricritical points, all other methods such as MC simulations [7, 10], series analysis [9], Transfer matrix calculations (TM) [3], renormalization group studies [11, 12] and mean field renormalization group approach [13] yield to the same phase diagram structure with only critical points. The whole phase diagram for the ATM was studied analytically by using the restricted ensembles method which is based on the Pirogov- Sinaï theory and its extension [7]. It was argued that the model presents a new phase called "$<\sigma>$" ($<\sigma>\neq 0$, $<S>=<\sigma S>=0$) on the line $K_2 = -K_4$ for $d > d_c$, where $d_c$ is a critical dimension. Using MC simulations and series expansion, Ditzian et al [10] have shown that $d_c = 3$ and the stability of this new phase extends around the line $K_2 = -K_4$. Whereas Migdal Kadanoff renormalization group procedure gives $d_c = 4$ [14] and shows that this "$<\sigma>$" phase is located at finite temperature and is characterised by an algebraic power law decay of the correlation function.

The anisotropic ATM was studied in d = 2 by using exact duality transformations and symmetry considerations [15]. It presents also partially ordered phases called $<\sigma>$ and $<S>$. These two phases are connected by symmetry operations to the $<\sigma S>$ phase. Recently, the transfer matrix technics [16] have shown that the critical exponents vary continuously along the Baxter-P phase transition. In order to study the effect of the crystalline anisotropy, an isotropic spin-1 ATM has been studied by using an effective field theory [17]. The phase diagram obtained, presents a rich variety of phase transitions which can be either of first or second order with multicritical and tricritical points. For strong values of the four coupling parameter $K_4$, the anisotropy interaction induces a new partially ordered phase called $PO_2$ ($<\sigma> = <S> \neq 0$ and $<\sigma S> = 0$) which does not exist in the spin-½ ATM.

This paper is a review of already published studies [18, 19, 20]. In order to study the effect of the

 

coupling anisotropy, the crystallin field and the mixed spins on the structure of the phase diagrams of the ATM. We introduce a generalised Hamiltonian. In section 2, we define the model that we have investigated. In section 3, we give a brief description of the MC simulations and present our main results. Finally, we conclude in section 4.

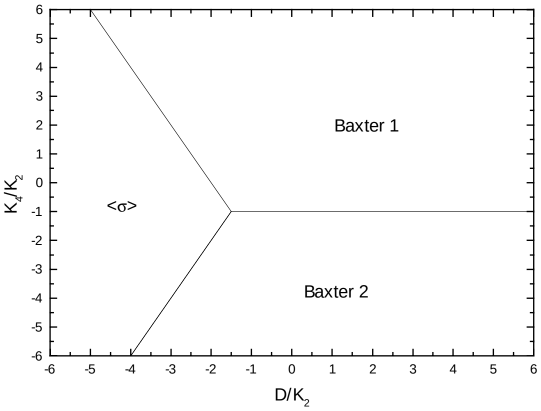


Fig. 1: Ground state phase diagram for mixed Ashkin- Teller model

## II. MODEL:

The generalisation of the ATM to a variety of models which describe two superposed spin systems is the following:

$$H = -K_2 \sum_{\langle i,j\rangle} \sigma_i \sigma_j - L_2 \sum_{\langle i,j\rangle} S_i S_j - K_4 \sum_{\langle i,j\rangle} \sigma_i \sigma_j S_i S_j - D \sum_i \left(\sigma_i^2 + S_i^2\right) \tag{2}$$

Where $\sigma_i$ and $S_i$ are spins localised on sites of an hypercubic lattice. The first (second) term describes the bilinear interaction between σ (S) spins, while the third term describes the four spin interaction. All these interactions are restricted to the z nearest-neighbour pairs of spins and there is on each site a single ion potential D.

When both spins σ and S take the values ±½ we recover the anisotropic spin-½ ATM which reduces in the invariant subspace $L_2 = K_2$ to the isotropic one. If both spins σ and S take the values ±1, 0, we obtain for $L_2 = K_2$ the isotropic spin-1 ATM. If mixed spins are used such that σ = ±½ and S = ±1, 0, the Hamiltonian (2) describes the isotropic mixed spin ATM for $L_2 = K_2$. For $K_4 = 0$, the Hamiltonian is reduced to two decoupled into two independent Ising spin-½ and Blume Capel [20] spin-1 models for σ = S = ±½ respectively σ = S = ±1, 0.

In order to calculate the ground state energy of the model, we express the Hamiltonian as a sum of the contributions of the pairs of nearest neighbours. Then the contribution of the pair $S_1$, $S_2$ and $\sigma_1$, $\sigma_2$ is:

$$E_P = -K_2\sigma_1\sigma_2 - L_2 S_1 S_2 - K_4 \sigma_1\sigma_2 S_1 S_2 - \frac{2D}{z}\left(S_1^2 + S_2^2 + \sigma_1^2 + \sigma_1^2\right) \tag{3}$$

where z is the coordination number (z = 4 for a square lattice)

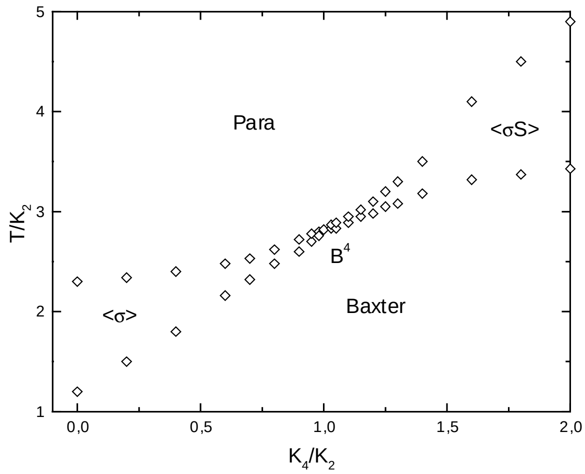


Fig. 2: Phase diagram as obtained from MC simulations in d=2 and L=30 for $L_2/K_2$=0.5. The diamonds denote second-order phase transitions. The meeting of all critical lines is located at the multicritical points $B^4$.

By comparing the values of Ep for different configurations we obtain the structure of the phase diagram at T = 0 [18, 20]. We notice that a partially ordered ferromagnetic phase which doesn't occur in the isotropic ATM only at line $K_2 = 0$ for $K_4 > 0$ have got a large region of stability which depends on the values of the ratios $K_4/K_2$, $L_2/K_2$ and $D/K_2$. To show that, we will give as an example the ground state phase diagram of the isotropic mixed spins ATM. (Fig. 1)

i) For $D/K_2 \geq -3z/8$: if $K_4/K_2 > -1$ the Baxter1 phase is stable since both spins $\sigma_i$ and $S_i$ are aligned, otherwise if $K_4/K_2 < -1$ the spins $\sigma_i$ are antiparallel while the spins $S_i$ are parallel then we have $\langle\sigma\rangle_F = \langle S\rangle_{AF} = \langle\sigma S\rangle_F = 0$, $\langle\sigma\rangle_{AF} \neq 0$, $\langle S\rangle_F \neq 0$ and $\langle\sigma S\rangle_{AF} \neq 0$ which characterise the phase called Baxter2.

ii) For $D/K_2 < -3z/8$: We have two critical values of single ion potential D, $D_{C_1}/K_2 = -z/4\,(1 - K_4/2K_2)$ and $D_{C_2}/K_2 = -z/2\,(1 + K_4/4K_2)$, such that if $D/K_2 < D_{C_1}/K_2$ and $D/K_2 > D_{C_2}/K_2$ the Baxter2 and Baxter1 phases are stable respectively. If $D_{C_1}/K_2 < D/K_2 < D_{C_2}/K_2$ the spins $\sigma_i$ are parallel while the spins $S_i$ are equal to zero then we have $\langle\sigma\rangle_F \neq 0$, and $\langle S\rangle_F = \langle\sigma S\rangle_F = 0$

thus we obtain the partially ordered phase called " <σ> ".

## III. MONTE-CARLO SIMULATIONS AND RESULTS:

We have performed MC simulations to complement transfer-matrix finite-size-scaling (TMFSS) calculations [16,19], and to compare the results with those obtained within a mean-field-approximation MFA [18, 20].The system studied is $L^d$ hypercubic lattice with even values of L, containing $N = L^d$ spins, where L is the linear size of the system. We use the well-known Metropolis algorithm [22] with periodic boundary conditions to update the lattice configurations. The physical quantities of use are the magnetizations $|M_\alpha|$ ($\alpha = \sigma$, S, $\sigma$S) and are estimated by :

$$|M_\alpha| = \langle |M_\alpha| \rangle = \frac{1}{N\varsigma} \sum_c \sum_i \alpha_i(c) \quad \text{with } \alpha = \sigma, S, \sigma S \quad (4)$$

where i runs over the lattice sites and c runs over the configurations obtained to update the lattice over one sweep of the entire N spins of the lattice (one Monte Carlo step, MCS) counted after the system reaches thermal equilibrium and ς is the number of the MCS.

In order to measure the phase boundaries we will find useful the measurement of fluctuations (variance of the order-parameter) in $M_\alpha$ defined by the magnetic susceptibility:

$$\chi_\alpha = \frac{N}{K_B T}\left(\langle M_\alpha^2 \rangle - \langle |M_\alpha| \rangle^2\right) \quad \text{with } \alpha = \sigma, S, \sigma S \quad (5)$$

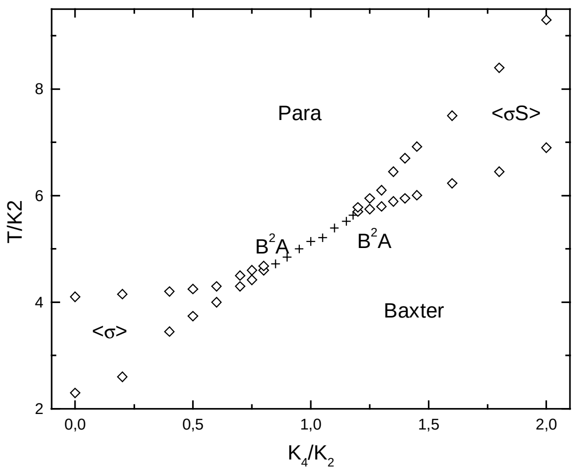


Fig. 3: Phase diagram as obtained from MC simulations for d=3 and for $L_2/K_2 = 0.5$. Diamonds and + denote second order respectively first order phase transitions. There are two multicritical points $B^2A$.

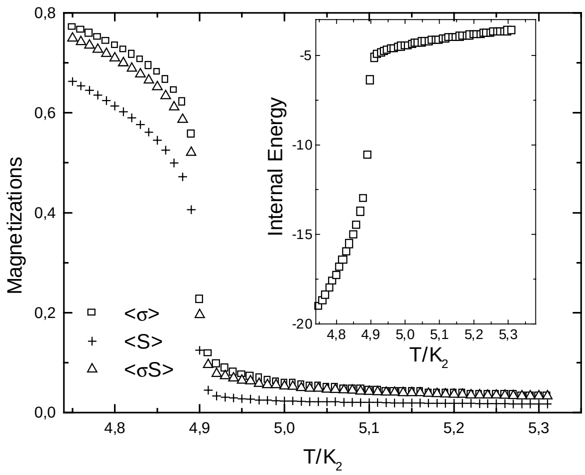


Fig. 4: Plot, for $L_2/K_2 = 0.5$ $K_4/K_2 = 0.95$, of the order-parameters <σ> and <S> = <σS> and the internal energy (inset) as obtained by MC simulation in d=3. Discontnuities are seen indicating first-order phase transition

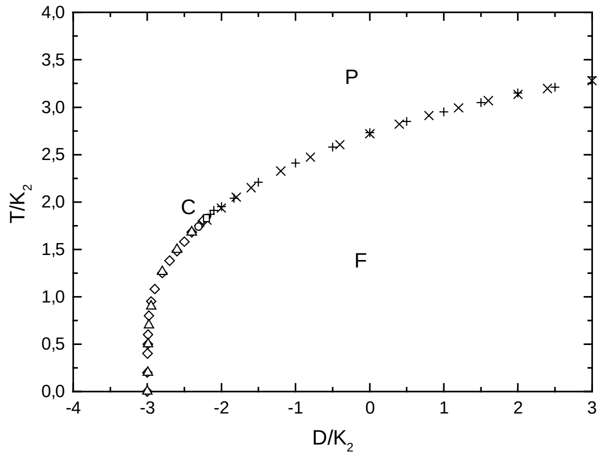


Fig. 5: The phase diagram in the $D/K_2$, $T/K_2$ plane for $K_4/K_2 = 1.0$, from Monte-Carlo (MC) and transfer-matrix (TM) data [14], is shown. TM results from scaling (the 2/3 data are not shown for clarity) where × and Δ denote respectively second and first-order transitions. A tricritical point is located at (o) $C_{TM}(-2.3 \pm 0.1, 1.738 \pm 0.001)$ from 3/4 scaling. MC data are also shown with L=30 (d = 2) where + ( ) denote second (first) order transitions. The MC tricritical point is ( ) $C_{MC}(-2.2 \pm 0.1,\ 1.82 \pm 0.01)$

The nature of phase transitions is determined by using the internal energy E = < H > and the order parameters. Then at second (first) order phase transition both internal energy and order parameters are continuous (discontinuous) [10, 23].

The symmetry of the spin-½ ATM under permutation σ↔S is broken when the anisotropy ($K_2 \neq L_2$) is introduced. However it can be restored by using the permutation $K_2 \leftrightarrow L_2$, the structure of the phase diagrams is then invariant under this global symmetry. The existence of the anisotropy suggests new features in the phase diagrams depending on the critical values of $L_2/K_2$. For $L_2/K_2 < 1$, we have obtained from MC simulations on a two dimensional lattice (d = 2) only one variety of phase diagram Fig. 2. The Baxter phase is separated from the

paramagnetic phase by the two partially ordered phases <σ> and <σS> at low and high values of $K_4/K_2$ respectively. The critical temperatures are determined from the maxima of the susceptibility. Also in these simulations, neither hysteretic behaviour nor discontinuities in the order parameters or internal energy were found when crossing the critical lines [18]. Thus the nature of phase transition is always of second order for all values of $L_2/K_2$. Our results are in good agreement with those obtained recently by transfer matrix Finite Size Scaling (TMFSS) calculations [16] and are close to those obtained exactly by Wu et al [15]. All these three exact methods yield only one multicritical point $B^4$. On the other hand, for $K_4/K_2 = 1$, the exponent estimates from TMFSS calculations have shown that this multicritical point is non universal. It belongs to the line $K_4/K_2 = 1$ with non universal and varying critical exponents. It is linked by two ends, from an Ising like one at $L_2/K_2 = 0$

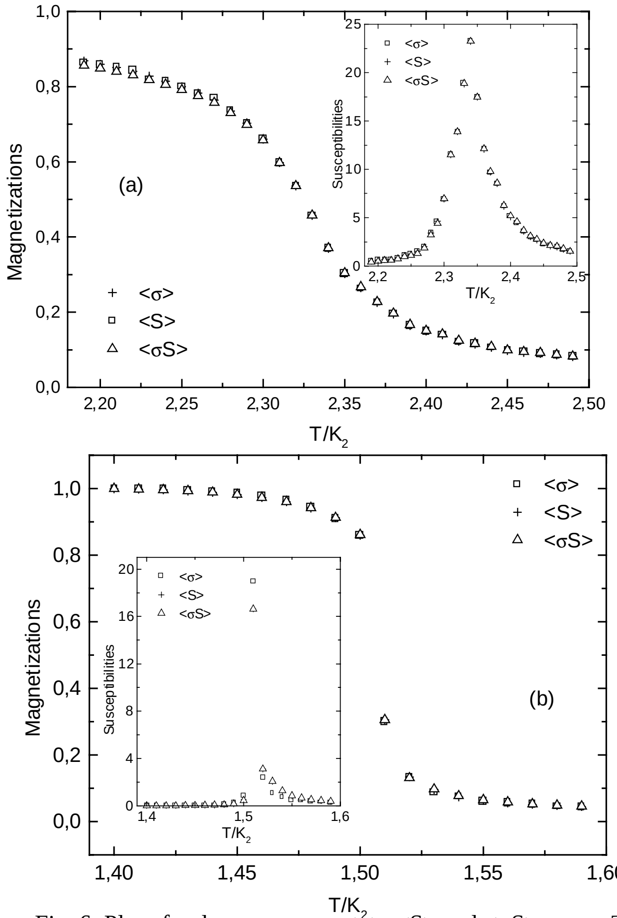


Fig. 6: Plot of order parameters <σ>, <S> and <σS> versus $T/K_2$ for $K_4/K_2$=1 and two values of the cristalline anisotropy from MC simulations with L=30 show that there is only one transition. The corresponding inset shows associated susceptibilities. (a) $D/K_2$= 1.0, the three order parameters are continuous indicating that the transition is of second-order. (b) $D/K_2$= -2.5, the three order parameters are discontinuous indicating that the transition is of first-order.

to the other one at $L_2/K_2 = 1$ which is the four state Potts model exponent [16].

We have also performed MC simulations for d = 3. The MFA [18] gives for $L_2/K_2 < 1$ four varieties of phase diagrams while the MC simulations reduce them to one type for all values of $L_2/K_2$. However the phase transition from the Baxter to paramagnetic phase, which is located on a multicritical point for d = 2, extends to a critical line which is of the first order Fig. 3 indicated by the discontinuities observed in the order parameter and the internal energy (Fig. 4). The critical lines separating the <σ> (<σS>) phase from the paramagnetic and Baxter phase remain of second order, thus yielding two critical end points in the phase diagram. For $L_2/K_2 = 1$ we recover the phase diagram of the ferromagnetic isotropic spin-½ ATM where the <σ> phase disappears while for $L_2/K_2 > 1$ it is obtained by using the symmetry between σ and S.

It is known that the criticallin line field influences on the orientation of the magnetic moments. The Blume-Emery-Griffiths model [21] is a simple model which enables a study of the effect of a such cristallin anisotropy. It has a richness of

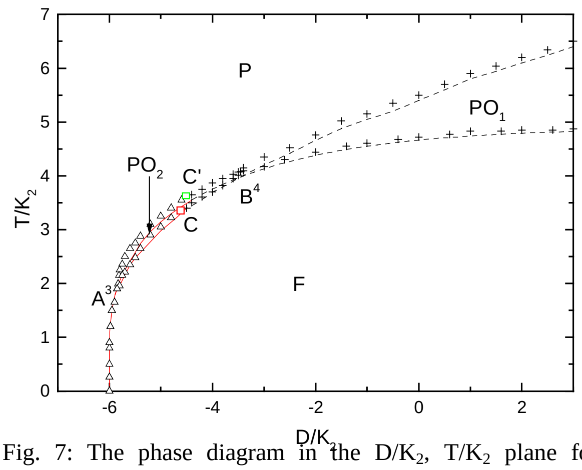


Fig. 7: The phase diagram in the $D/K_2$, $T/K_2$ plane for $K_4/K_2$=4.0, from Monte-Carlo (MC) and transfer-matrix (TM) data, is shown. The solid lines (first-order transition) and dashed lines (second-order transition) are the TM results from 2/3 scaling. Tricritical, multicritical and triple points are located espectivelyat $C_{TM}(-4.5\pm0.1, 3.4\pm0.001)$ $C'_{TM}(-4.4\pm0.01, 3.551\pm0.001)$, $B^4_{TM}(-3.5\pm0.1, 3.95\pm0.001)$ and $A^3_{TM}(-5.88\pm0.02, 1.8\pm0.1)$ from 2/3 scaling. MC data are also shown with L=30 (d = 2) where + (◊) denote second (first) order transitions. The MC tricritical, multicritical and triple points are located respectively at( ) $C_{MC}(-4.6\pm0.1, 3.35\pm0.01)$ ,( ) $C'_{MC}(-4.5\pm0.01, 3.62\pm0.01)$ ( ), $B^4_{MC}(-3.45\pm0.05, 4.08\pm0.01)$ and $A^3_{MC}(-5.85\pm0.02, 1.9\pm0.1)$.

properties such as critical , tricritical and first order transitions [24]. In order to study the crystalline anisotropy on the Ashkin-Teller spin systems we consider the isotropic ($K_2 = L_2$) spin-1 ATM. However the spin variables $\sigma_i$ and $S_i$ have both a magnitude of one (σ = S = ±1, 0) then the model (eq 2) allows a single ion-potential D.

Using MC simulations for d = 2 we show that the anisotropy parameter introduces a new partially ordered phases and rich variety of critical frontiers. For $\alpha = K_4/K_2 < \alpha_c$ (critical value of $K_4/K_2$) the system exhibits only a phase transitions between ferromagnetic (Baxter) phase (F) and paramagnetic phase. The critical line is of second order respectively first order for $\delta = D/K_2 > \delta^*(\alpha)$ respectively $\delta < \delta^*(\alpha)$ (Fig. 5). The two critical frontiers meet at the tricritical point C. The nature of transitions is determined from peaks in the persistence length using TMFSS [16] and from discontinuities (continuities) and hysterisis behaviour in the order parameters for first (second) order transitions using MC simulations [14] (Fig. 6a-b). We mention that MC results are in excellent agreement with those obtained from TM [19] and qualitatively better than those obtained from the EFT [17]. By increasing the value of $\alpha$, $\alpha > \alpha_c$, all phase sinks within different topologies appear then the model exhibits in one hand a partially ordered phases called $PO_1$ and $PO_2$ and in other hand different critical frontiers and higher order critical points. Our results from MC and TM [19] data are plotted in Fig. 7 for $\alpha = 4$. The partially ordered phase $PO_1$ characterised by $<\sigma> = <S> = 0$ and $<\sigma S> \neq 0$

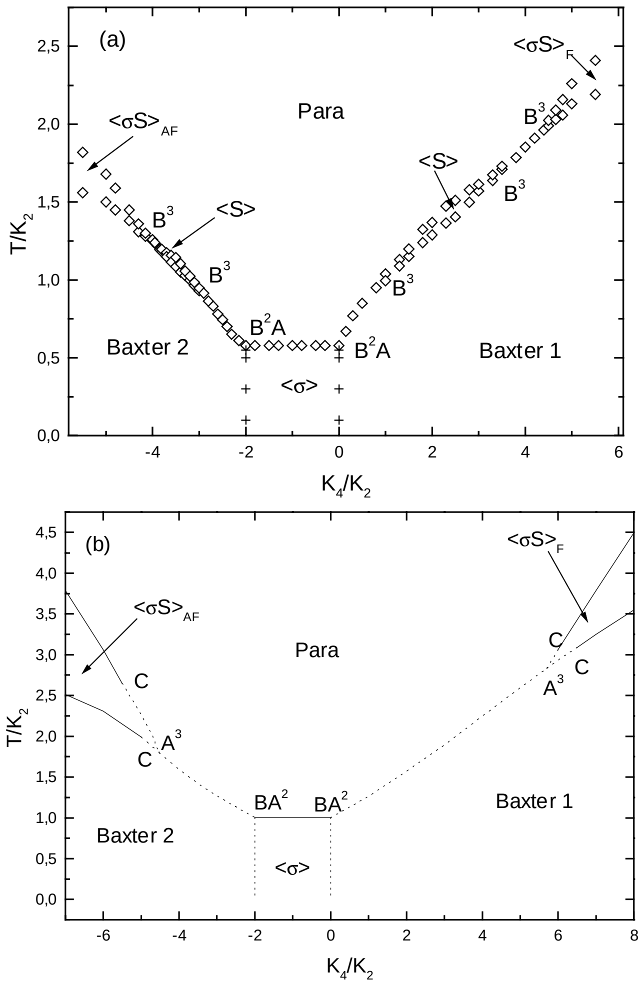


Fig. 8: Phase diagram for $D/K_2 = -2$ as obtained from: (a) Monte Carlo simulations in d = 2, where diamonds and plus denote second and first order phase transitions respectively. There is multicritical point $B^3$ and critical end points $B^2A$. (b) Mean field approximation. Solid and dashed lines denote second and first order phase transitions respectively. In the phase diagram, it occurs tricritical points C, triple points $A^3$ and critical end points $BA^2$.

appears at high anisotropy $\delta = D/K_2$. It is the usual partially ordered phase of the spin-½ ATM. It is bounded by lines of second-order which separate the paramagnetic and ferromagnetic phases. By decreasing the crystal field, a new partially ordered phase, $PO_2$ characterised by $<\sigma> = <S> \neq 0$ and $<\sigma S> = 0$, appears at high temperature and separates the ferromagnetic phase from the paramagnetic one by lines of second and first order transitions. These lines meet at tricritical points C and C' (Fig. 7). At low temperature the two first order lines meet at a triple point $A^3$ and melt into a critical line of first order which separates the paramagnetic and ferromagnetic phases. The regions of stability of the four phase sinks meet at a multicritical point $B^4$. Contrarily to the EFT which gives five varieties of phase diagrams [15], the MC simulations reduces them to one. Then by increasing the value of $\alpha = K_4/K_2$ we observe a migration of the tricritical and multicritical points to higher anisotropy values.

The transfer-matrix Finite-Size-Scaling estimates of the exponent $\nu$ [19] have shown that for $\alpha = 1$, we have a line of critical points which belong to the four state Potts model for a range of values of the anisotropy, instead of only one point of the four state Potts model in the spin-½ ATM. At lower $D/K_2$, the model falls into the Ising tricritical universality class. When the coupling $K_4/K_2$ becomes strong, $\alpha > 2$, the exponents calculations show that the critical lines separating the F-$PO_1$-P and F-$PO_2$-P phases belong to the Ising critical and tricritical universality classes [19].

In order to study the effect of mixed spins on the structure of phase diagram we assume that the spins $\sigma_i$ and $S_i$ which are localised on each site of an hypercubic lattice take respectively the values $\sigma_i = \pm 1/2$ and $S_i = \pm 1, 0$. Our MC results are presented for d = 2, in the plane ($K_4/K_2$, $T/K_2$). The model exhibits a rich variety of phase transitions which meet at a multicritical points (Fig. 8a). At high temperature the ordered phases Baxter1 and Baxter2 are separated respectively from the paramagnetic phase by the partially ordered phases $<\sigma S>_F$ and $<\sigma S>_{AF}$ at high absolute values of $K_4/K_2$. At intermediate absolute values of $K_4/K_2$, the MC results present a new partially ordered phase "<S>" , while within a MF approximation it doesn't occur Fig. 8b [20]. We remark that this new phase define $<\sigma> = <\sigma S> = 0$

and <S> ≠ 0,doesn't exist neither in the ferromagnetic spin-½ [10] nor in the spin-1 AT models. However, the symmetry of this model under permutation σ ↔ S is broken. Then if we increase the temperature at intermediate values of $K_4/K_2$ we disorder the spins σ at first while the spins S remain ordered and the system stabilises at intermediate values of the temperature into this new phase <S>. The critical lines are all of second order and linked by a multicritical points $B^3$ and $B^2A$.

## IV. CONCLUSION:

In this paper, we have generalised spin-½ Ashkin-Teller model which describes a four component systems to a large variety of models. We have studied, using MC simulations, The effects of the coupling anisotropy, the crystalline anisotropy and the mixed spins on the structure of the phase diagrams. We have shown that those models exhibit a rich varieties of phase diagrams and present new partially ordered phases for d ≥ 2. The nature of those new phases which don't occur in spin-½ ATM for d = 2 depends on the nature of the model. The critical lines for the anisotropic spin-½ ATM are all of second order as confirmed recently by TMFSS calculations of the exponent ν, while for the spin-1 ATM and the mixed spin ATM the phase diagrams exhibit critical lines either of first or second order with tricritical and multicritical points. For spin-1 ATM by using TMFSS [19] calculations we have shown, for α = 1, that the thermal exponent ν at the phase transition Baxter-P belongs to the four-state Potts model universality class and falls into an Ising tricritical point for low values of $D/K_2$. Whereas for high values of $K_4/K_2$, all the critical lines P-$PO_2$ and F-$PO_1$ are Ising-like phase transitions.

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