Study of the Ashkin Teller model with spins $S = 1$ and $\sigma = 3/2$ subjected to different crystal fields using the Monte-Carlo method

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Using the Monte-Carlo method, we study the magnetic properties of the Ashkin-Teller model (ATM) under the effect of the crystal field with spins $S = 1$ and $\sigma = 3/2$. First, we determine the most stable phases in the phase diagrams at temperature $T = 0$ using exact calculations. For higher temperatures, we use the Monte-Carlo simulation. We have found rich phase diagrams with the ordered phases: a Baxter 3/2 and a Baxter 1/2 phases in addition to a $\langle rS \rangle$ phase that does not show up either in ATM spin 1 or in ATM spin 3/2 and, lastly, a $\langle r \rangle = 1/2$ phase with first and second order transitions.

Key words: Ising model, Ashkin-Teller, spin-1, spin-3/2, Monte Carlo

1. Introduction

In recent years, the functioning of spins in different network structures has been a magnetic manifestation. It also allowed one to verify the nature of the phase transition as well as the critical behavior in the field of statistical mechanics [1]. In addition, the properties of magnetic materials and their technological applications such as thermomagnetic recording media and micro-electromechanical systems are characterized by the phenomenon of mixed spins, which are well defined in the Ising model approach [3]. Studies of magnetic materials of mixed spins have been extended to the Ising model in the presence of a crystalline field and, specifically, are applied to the mixed spin (1, 3/2). The latter studies have shown some interesting behaviors using an effective field theory. The results of the field theory study have shown that the mixed spin system has first order transition lines as well as offers tricritical and triple points. They also found out that the system is of the types [3]. However, in the context of mixed spin (1, 3/2), the Blume-Capel Ising model was realized when a first order transition line was found separating two ferromagnetic regions on a square cubic lattice [5]. Using Monte Carlo simulations, it was shown that the interactions between the nearest neighbors of the Ising model $J_1$, $J_2$ and $J_3$ with frustrations are the main barriers to the transmission change in the increase in temperature and also indicate an Ashkin-Teller behavior. This study estimates the transition points at the critical point of Potts and confirms the first order transition behavior in the stabilization state of $J_1$ antiferromagnetic [6]. In addition, they conducted studies on the nature of the four-stage thermal phase transition degraded in a Monte Carlo simulation and the finite size scaling. On the other hand, first-order behaviors are noted under Potts’ critical points with four states, and thus, his work indicates that the four-state transition in the Ising anti-magnetic model represents a similar transition [7]. In this context and to properly describe the notion of phase transitions, Ashkin and Teller [8] developed a very interesting model in these Ising systems and, thus, simplified the study of statistical mechanics. In this model, one could introduce the
2. Model and phase diagram of the fundamental state

In this work, we consider the Ashkin-Teller model in the case of mixed spins $\sigma = 3/2$ and $S = 1$. We analyze this case under the effect of different crystal fields. Thus, this model is described by the following Hamiltonian:

\[ H = -K_2 \sum_{\langle i,j \rangle} (\sigma_i \sigma_j + S_i S_j) - K_4 \sum_{\langle i,j \rangle} \sigma_i \sigma_j S_i S_j - D_1 \sum_i S_i^3 - D_2 \sum_i \sigma_i^2, \]  

where the variables $\sigma_i$ and $S_i$ take the values $(\pm 3/2, \pm 1/2)$ and $(\pm 1, 0)$, respectively, and are located on the sites of a cubic lattice, $\langle i, j \rangle$ refers to a pair of nearest neighbor spins. The first term of equation (2.1) refers to the bilinear interactions between the spins located at the sites $i$ and $j$ using the coupling parameter $K_2$. Moreover, the second term refers to the interaction of the four spins with the coupling constant $K_4$. The last term refers to the existence of two ionic crystal fields $D_1$ and $D_2$. From the contribution of a pair of $S_1, S_2, \sigma_1$ and $\sigma_2$, the Hamiltonian is expressed as a sum of contributions of the nearest neighbors, we obtain the pair energy as follows:

\[ E_p = -K_2 [ (\sigma_1 \sigma_2) + S_1 S_2 ] - K_4 (\sigma_1 \sigma_2 S_1 S_2) - D_1 \frac{1}{2} (S_1^2 + S_2^2) - D_2 \frac{1}{2} (\sigma_1^2 + \sigma_2^2). \]
Study of the Ashkin Teller model with spins $S = 1$ and $\sigma = 3/2$ subjected to different crystal fields

According to the values containing the variables $S_i$ and $\sigma_i$, we extract 144 ($3^2 \times 4^2$) possible configurations for the ground state at $T = 0$. Using symmetry configurations, this number reduces to 24 configurations. For each set of parameters: $K_2, K_4, D_1$ and $D_2$, we select the configuration with minimal energy $E_p$. This leads to the phase diagram in the fundamental state ($T = 0$). Different phases will be given in the form $(S_1, \sigma_1, S_2, \sigma_2)$. In what follows, we consider different situations by fixing one parameter and varying the others (the latters will be normalized by $K_2$). In figure 1, we plot the phase diagram by varying the parameter $K_4/K_2$ as a function of $D_2/K_2$ (letting $D_1 = 0$):

- For $D_2/K_2 < -1$, if $K_4/K_2 < -1$ and $K_4/K_2 > D_2/K_2 + 1/4$: we observe that the $S_i$ spins are parallel such that $\langle S_i \rangle = 1$ and $\sigma_i$ spins are antiparallel. Consequently, the stable phase obtained is the antiferromagnetic phase. For $K_4/K_2 > -1$ and $K_4/K_2 > -D_2/K_2 - 1$. We can distinguish that the spins $S_i$ and $\sigma_i$ are both aligned in the same direction, so $\langle \sigma S \rangle = 1/2$; this corresponds to the ferromagnetic phase.

- In the case: $D_2/K_2 > -1$, if $K_4/K_2 < -4/9$, we can observe that the $\sigma_i$ spins are parallel such that $\langle \sigma \rangle = 3/2$ and $S_i$ spins are antiparallel. Consequently, the stable phase obtained is the antiferromagnetic phase. Otherwise if $K_4/K_2 > -1$ and $K_4/K_2 > -D_2/K_2 - 1$. We can distinguish that the spins $S_i$ and $\sigma_i$ are both aligned in the same direction, including $\langle S \rangle = 1$ and $\langle \sigma \rangle = 3/2$ so $\langle \sigma S \rangle = 3/2$ while we have the ferromagnetic phase 3/2.

In the second situation, we obtain the figure which represents the variation of $K_4/K_2$ as a function of $D_1/K_2$. Lastly, we put $D_1 = D_2 = D$ and draw the diagram $K_4/K_2$ as a function of $D/K_2$ (figure 2).

Figure 1. Phase diagram of the fundamental state in the case of $D_1 = 0$.

Figure 2. Phase diagram of the fundamental state in the case $D_1 = D_2 = D$. 

33707-3
Figure 3. Phase diagram of the fundamental state in the case of $D_2 = 0$.

Figure 3 shows a phase diagram in the fundamental state and parameter variation $K_4$ as a function of crystalline field $D_1$ ($D_2 = 0$).

This figure shows a phase diagram in the fundamental state and parameter variation $K_4$ as a function of crystalline field $D_1$ ($D_2 = 0$):

- For $D_1/K_2 < -0.1$ or $K_4/K_2 > 4/9D_1/K_2 - 4/9$ and $K_4/K_2 > -4/9D_1/K_2 - 4/9$: we have a stable phase called the phase $\langle \sigma \rangle$ because we have the spins $S_i$ being equal to zero such that $\langle S \rangle = \langle \sigma S \rangle = 0$ and $\langle \sigma \rangle = -3/2$.

- For $D_2/K_2 > -0.1$, if $K_4/K_2 > -4/9$ and $K_4/K_2 > -D_2/K_2 - 1$: we observe that the $S_i$ spins are parallel such that $\langle S \rangle = 1$ so that the $\sigma_i$ spins are antiparallel or $\langle \sigma \rangle = 3/2$, consequently the stable phase obtained is the antiferromagnetic phase. Otherwise if $K_4/K_2 > -1$ and $K_4/K_2 > -D_2/K_2 - 1$.

We can observe that the spins $S_i$ and $\sigma_i$ are both aligned in the same direction, including $\langle S \rangle = 1$ and $\langle \sigma \rangle = 3/2$ so $\langle \sigma S \rangle = 3/2$ while we have the ferromagnetic phase $3/2$ as the stable phase.

The third case was made using $D_1 = D_2 = D$ (figure 2). We draw the diagram $K_4$ according to crystalline field $D$ such that:

- For $K_4/K_2 > -12/9D/K_2 - 12/9$ and $K_4/K_2 > -0.4$; we have $\langle \sigma \rangle = 3/2$, $\langle S \rangle = 1$ and $\langle \sigma S \rangle = 3/2$ so $\langle \sigma \rangle = \langle \sigma S \rangle$ such that the spins $\sigma_i$ and $S_i$ are both parallel, then we have the Baxter $3/2$ phase called the ferromagnetic Baxter phase (the stable phase).

- For $K_4/K_2 < 4/9D/K_2 - 4/9$ and $K_4/K_2 < -0.4$; in this part of the diagram we see that the spins $\sigma_i$ are parallel so that the spins $S_i$ are antiparallel. This means that we have an antiferromagnetic Baxter phase, which is always the Baxter phase (3/2).

- For $K_4/K_2 < -12/9D/K_2 - 12/9$ and $K_4/K_2 > 12/9D/K_2 + 4/9$, in this region we have $\langle \sigma \rangle = 1/2$ and $\langle S \rangle = 0 = \langle \sigma S \rangle = 0$, so the phase here is the phase symbolized by $\langle \sigma \rangle$, because the spins $S_i$ are equal to zero and the spins $\sigma_i$ while the parallel ones designate phase $1/2$.

- For the zone that is noticed in the phase diagram and which is specified by the equations: $K_4/K_2 > 4/9D/K_2 - 4/9$ and $K_4/K_2 < -4/9D/K_2 - 4/9$ and if $D = -1$, we have the spins $\langle S \rangle = 0$ and $\langle \sigma \rangle = 3/2$, such that $S_i$ are equal to zero and $\sigma_i$ are parallel. Finally, we obtain the phase $\langle \sigma \rangle$ is the phase $\langle \sigma \rangle = 3/2$ which does not exist either in the case of mixed spin $-1/2$ or in the Ashkin-Teller model for spin-$3/2$.

3. The Monte Carlo simulation

In our work, to determine the magnetic properties of the Ashkin-Teller model for non-zero temperatures, we use Monte Carlo simulations implemented with the Metropolis algorithm with periodic boundary conditions to update the lattice configurations. We consider a 2d square lattice of $L \times L$ size.
which contains $N = L^2$ sites. We performed the simulations for system size $L = 30$. We performed simulations for certain values of the parameters $K_d$, $D_1$ and $D_2$ using $P = 100000$ Monte Carlo steps after discarding the first 20000 MCS for thermal equilibrium. The magnetization of the system is given by the formula:

$$|M_{\alpha}| = \langle |M_{\alpha}| \rangle = \frac{1}{N_P} \sum_c \sum_i a_i(c)$$

(3.1)

with $\alpha = \sigma, S, \sigma S$, where $i$ runs over the lattice sites and $c$ runs over the obtained system configurations obtained. The lattice is updated by a sweep of the $N$ spins (the Monte Carlo step) after the system reaches thermal equilibrium. The magnetic susceptibility relationship is given by:

$$\chi_{\alpha} = N/(K_B T) \left( \langle M_{\alpha}^2 \rangle - \langle |M_{\alpha}| \rangle^2 \right)$$

(3.2)

with $\alpha = \sigma, S, \sigma S$ and the Binder cumulant is given by:

$$U_{\alpha} = 1 - \frac{\langle M_{\alpha}^4 \rangle}{3 \langle M_{\alpha}^2 \rangle^2}.$$  

(3.3)

Errors are deducted from the blocking method.

### 4. Results and discussions

We obtain the magnetization behavior as a function of temperature as well as the susceptibilities of the studied system for different values of the coupling parameters. As shown in figure 4 our MC results at low temperature show a ferromagnetic Baxter phase $(S_1 \sigma_1 S_2 \sigma_2) = (1 \ 3/2 \ 1 \ 3/2)$ with $\langle \sigma S \rangle = 3/2$ (figure 4a) and a ferromagnetic Baxter phase $(1 \ 1/2 \ 1 \ 1/2)$ with $\langle \sigma S \rangle = 1/2$ (figure 4b) as expected from the $T = 0$ phase diagram (figure 1), where we find a new partially ordered phase $(\sigma S)$ identified by $\langle \sigma \rangle = \langle S \rangle = 0$, and $\langle \sigma S \rangle \neq 0$. For high temperatures in both cases, the system becomes disordered. The critical transition temperature is estimated from the maximum of the susceptibility associated with the different magnetization. We found for the case (a) $T_c = 7.39$ and for case (b) $T_c = 1.89$. In addition, the transition between the phases mentioned is always of second order due to the continuity of the order parameters across the transition line. In figure 5 the first case (a) at low temperature, we have $\langle \sigma \rangle = 1/2$, $\langle S \rangle = \langle \sigma S \rangle = 0$ corresponds to the phase $(0 \ 1/2 \ 0 \ 1/2)$. However, at high temperature the system undergoes a transition to the paramagnetic phase. For the second case (b) $D = -2$ and $K_d = 3$, the ground...
Figure 5. (Colour online) The magnetization (for the parameters \(\sigma\), \(S\), \(\sigma S\)) as a function of the temperature, with system size \(L = 30\), with crystal field \(D_1 = D_2 = D\), in the two cases a) \(K_4 = 1\), \(D = -6\) and b) \(K_4 = 3\), \(D = -2\) a partially ordered is observed at high temperature.

Figure 6. (Colour online) Phase diagram in the plane \((D_2/K_2, T/K_2)\) for \(K_4 = 1\) by MC simulation with \(L = 30\).

The state is the ferromagnetic Baxter phase (1 3/2 1 3/2). The susceptibility plot shows a peak corresponding to \(\langle \sigma \rangle\) and \(\langle S \rangle\) at the critical temperature \(T_{c1} = 11.09\); by contrast, the susceptibility corresponding to \(\langle \sigma S \rangle\) shows a distinct peak at the transition temperature \(T_{c2} = 14.19\), clearly defining a partially ordered phase \(\langle \sigma S \rangle\) at high temperature separating the disordered phase from the Baxter phase.

The phase diagram in figure 6 shows the stable phases at different temperature in the plane \((D_2/K_2, T/K_2)\) in the case \(D_1 = 0\) for the coupling parameter \(K_4 = 1\), we found that for low values of \(D_2/K_2\), two phases are separated by a first order transition line. This is shown in figure 8. The verification of the phase transition nature is determined from the discontinuity or continuity of the order parameters [25]. The two phases are: ferromagnetic Baxter 1/2 and ferromagnetic Baxter 3/2. The former phase \(\langle \sigma \rangle = 1/2\) was neither found for this ATM model with spin-1/2 [9] nor in the Ashkin-Teller model with spin-3/2 [26]. At high temperature, a second order transition to the paramagnetic disorder phase takes place. The Baxter ferromagnetic-3/2 is stable for large values of \(D_2/K_2\).

In figure 7 we plot the phase diagram in the \((T/K_2, D/K_2)\) plane. We found out a similar form of the phase diagram as in figure 6 except that the low temperature low \(D\) phase is now \(\langle \sigma \rangle = 1/2\) phase with a first transition line to the ferromagnetic Baxter 3/2 for large values of \(D\). We also note that the \(\sigma - 1/2\) phase was not found in the Ashkin-Teller for spin-3/2 [26]. Moreover, when the coupling parameter values are increased \(K_4/K_2 = 3\) for the case of \(D_1 = D_2 = D\) with the growth of the values of \(D/K_2\). In figure 9 we found out a partially ordered \(\langle \sigma S \rangle\) phase, figure 5b, between the ordered phase of Baxter ferromagnetic
Study of the Ashkin Teller model with spins $S = 1$ and $\sigma = 3/2$ subjected to different crystal fields

3/2 and the disordered paramagnetic phase at high temperature. These phases were illustrated in previous cases (figure 6). This new phase $\langle \sigma S \rangle$ was also found in the model Ashkin-Teller mixed of spin-1/2 [13] but not in the Ashkin-Teller for spin-3/2 [26]. By decreasing the crystal field $D/K_2$, we found a transition from Baxter ferromagnetic 3/2 to the paramagnetic phase which is of first order type. We also observe the same phase $\langle \sigma \rangle = 1/2$ as in figure 7 which separates high temperature paramagnetic phase in low values of $D/K_2$ by a second order transition, and is separated with a ferromagnetic Baxter 3/2 phase by a first order transition.

The phase transition points to a function of temperature at the fixed values of the coupling $K_4/K_2$ as well as the crystalline field $D_2/K_2$, which were pre-located from the points of intersection of the cumulative curves of Binder specified by the equation (3.3). We show these cases for $D_2/K_2 = 3$ ($D_1/K_2 = 0$) for different size of $L = (10, 20, 30, 40, 60)$ and the susceptibilities as a function of temperature as well as the Binder cumulant as a function of temperature figure 10 plotted. It is noted in figure 10 that the peaks when $L$ increases, show the transition point which means the critical temperature or the change of phase transition. Nevertheless, the Binder accumulate curves whose figure 10 shows that there is an intersection point that defines the critical temperature knowing that $T_c = 6.55$.

Figure 7. (Colour online) Phase diagram in the plane $(D/K_2, T/K_2)$ for $K_4 = 1$ by MC simulation with $L = 30$.

Figure 8. (Colour online) The magnetization (the parameters $\sigma$, $S$, $\sigma S$) as a function of the temperature with system size $L = 30$ with $T = 1$. 
5. Conclusion

In order to well describe the magnetic properties of Ising typical systems in statistical mechanics, and within this framework, we analyzed the Ashkin-Teller model with spins (1, 3/2) on a cubic lattice under the effect of different crystalline fields and the coupling parameters which are defined in equation (2.1). The first step of our study was the most important of the stable phase in the fundamental state (zero temperature) in three cases of crystalline field; the system undergoes a first-order phase transition between these stable phases because we noticed that we have phases that did not exist in ATM spin-1/2. On the other hand, when the temperature is non-zero, we have processed the AT model by the Monte Carlo simulation, specifically, using the Metropolis method. As a result, we found out that the coupling parameter values were fixed and the crystal field varied with the temperature variation. We also found out that we had the second-order phase diagram, which contained stable phases such as the Baxter phase 3/2 as well as the paramagnetic phase in different cases of crystalline field in the parameter space \( \frac{K_4}{K_2}, \frac{D_1}{K_2}, \frac{D_2}{K_2}, \frac{D}{K_2}, \frac{T}{K_2} \) delimited by lines with multicritical points. Crucially, we found a new phase in the phase diagram in space \( \frac{K_4}{K_2}, \frac{D}{K_2}, \frac{T}{K_2} \). Finally, we verified the phase transition nature of this model, which is of second order phase transition of Ising type.
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Вивчення моделі Ашкіна-Теллера зі спінами $S = 1$ і $\sigma = 3/2$ під дією різних критичних полів із застосуванням методу Монте Карло

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Використовуючи метод Монте Карло, досліджено магнітні властивості моделі Ашкіна-Теллера (MAT) зі спінами $S = 1$ і $\sigma = 3/2$ під дією кристалічного поля. Спочатку визначено найстійкіші фази на фазових двідіаграмах при температурі $T = 0$ з допомогою точних обчислень. При вищих температурах ми використовуємо моделювання методом Монте Карло. Знайдено багато фазових двідіаграм із впорядкованими фазами: фазу Бахтера 3/2 і фазу Бахтера 1/2 додатково до фази $\langle \sigma S \rangle$, яка не з'являється ні в MAT зі спіном 1, ні в MAT зі спіном 3/2 і, нарешті, фазу $\langle \sigma \rangle = 1/2$ з переходами першого і другого роду.

Ключові слова: модель Ізінга, Ашкін-Теллер, спін-1, спін-3/2, Монте Карло