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ANTIPHASE PHENOMENA IN 2D ISING SQUARE LATTICE

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ABSTRACT:- *Monte Carlo simulations of the two dimensional Ising model were carried out to determine the impact of Antiphase Boundaries (APBs) in some thermodynamic functions of the system. We considered several lattice sizes and sometimes both Ferromagnetic (FM) and Antiferromagnetic (AFM) interactions for the same lattice. The analysis of the curves obtained shows that APBs appears only in AFM interaction and their effect is the creation of an energy gap that prevents the system from reaching the ground state. This happens only in lattices with odd linear size L (L = 9, 15, 31 …). However, these boundaries do not change the critical temperature of the Antiferromagnetic/Paramagnetic (AFM/PARA) phase transition which remains approximately at 2.26 (in unit of J/k_B). Nevertheless, they impose on the curve of the specific heat a jittery behaviour as a function of the temperature and with no clear peak as opposed to the case of even L (L = 16 ,20, 48,…) where there is a clear peak and a smooth curve. There is also a fluctuating magnetization around the value zero at low temperature (AFM phase). We show that this energy gap is proportional to 1/L where L is the linear size of the lattice, thus this gap should vanish if L becomes high. A similarity has been established with the role played by APB in some crystal structures and more especially in the binary alloys that are moreover described by the Ising model.*

INTRODUCTION

Crystal structures are described with the help of the Bravais lattices that classify them in systems according to the arrangement of atoms in the elementary cell. Nevertheless, the arrangement of atoms in most crystals is different from the one expected: the structure is said to present a fault. The faults affect considerably the general behaviour and properties of the material, but they are sometimes useful. Amongst two dimensional faults in solids, we can quote the Antiphase Boundaries (APBs) to which many works have been devoted. From the analysis of previous works [1-5] we can conclude that the influence of APBs on the properties (magnetic, mechanical…) of the materials depends strongly on the density of APBs [6] and on the temperature. In $Sr_2FeMoO_{6,}$ magnetization measurements revealed a slightly lowered saturation magnetization for the sample exhibiting the highest concentration of APBs as compared to samples with low concentration of APB atoms [5]. In the 18R Cu-Zn-Al alloy, the energy of the APB is proportional to the inverse of its width [1]. In particular, the width of the APB can increase with an increase in the temperature. An increase in the temperature is accompanied by an increase in the width of the boundary and a decrease in its energy. The phenomenon is called relaxation. Thus, the APB can be considered as a strengthening mechanism due to the gain of energy they cause. Since the binary alloys can be described by the Ising model, some phenomena such as APBs that happen in some solids should be observed and interpreted within the framework of that model. In general, problems in physics are solved using models and considering some approximations. In the Ising model, if we consider only the Antiferromagnetic (AFM) Nearest Neighbours (NN) interaction, Periodic Boundary Conditions (PBC) lead to the creation of an APB which is similar to a fault in comparison with the real AFM phase. Also, in some conditions, if we take into account the Next Nearest Neighbours (NNN) interaction, the Antiphase is obtained.

The purpose of the present work is not only to determine the impact of APB on some thermodynamic functions of the considered lattices, but also to provide a qualitative analogy between their characteristics in real materials and in the Ising model. Before we present the results of numerical simulations, we first recall some important notions on Ising model and on its equivalence with order-disorder phase transition in binary alloys.

ISING MODEL AND BINARY ALLOYS

The Ising Model [7]

The Ising model is obtained from the Heisenberg Hamiltonian in which it is considered that the Ferromagnetic (FM) state of spins is due to a quantum interaction called "exchange interaction". This Hamiltonian has the general form:

$$H_{ij} = -J_{ij}\overrightarrow{S_i}\overrightarrow{S_j} \quad (1)$$

In order to avoid difficulties related to the fact that the components of an operator of spin do not commute, only the spin component along one direction is considered in the Ising model. In addition, the interaction is considered to be isotropic and J_{ij} is therefore the same for all pairs of neighbouring spins: $J_{ij} \equiv j$.

$$H_{ij} = -JS_iS_j \quad (2)$$

Here, *J* is a positive number. This model is also used to study antiferromagnetism, *J* being negative in this case.

Phase Transition In The Ising Model

Onsager in 1944 [8] showed that for a square lattice, a phase transition occurs in the two dimensional Ising model at the critical temperature T_c given by:

$$T_C = \frac{2J}{k_B \ln\left(1+\sqrt{2}\right)} \quad (3)$$

Or $$T_C = 2,26\left(J/k_B\right) \quad (4)$$

We recall that there is no phase transition in the one dimensional model and that there is no analytic solution for the three dimensional model until now. The energy of the system has its minimum value when all spins are pointed in the same direction (up-up) for FM interaction or in opposite direction (up-down) for AFM interaction. The interaction energy of a central spin with its four nearest neighbours is given by:

$$\mathrm{E} = -\ 4\mathrm{J}\times\frac{1}{2} = -2\mathrm{J} \quad (5)$$

The factor 1/2 is introduced in order to avoid the double counting between nearest neighbours. In unit of $\left|J\right|/k_BT$, this energy is equal to $\square 2$. For L×L lattice size, this energy is $\square 2(L)^2$. Thus, the energy per spin is $\square 2$. A similar calculation leads to the same value for antiferromagnetic interaction with *J<0*.

The order parameter in Ferromagnetic/Paramagnetic (FM/PARA) phase transition is the magnetization. This is because the magnetization vanishes in PARA phase (high temperature) and differs from zero in FM phase (low temperature). But the magnetization is no longer the order parameter in AFM/PARA transition because it has a zero value in the two phases. Here, one should rather consider the difference between the magnetizations of the two antiparallel sublattices constituting the whole lattice as the order parameter.

The heat capacity and the susceptibility are linked respectively to the fluctuations of the energy and the magnetization. Thus they can be written in the form:

$$C_v = \frac{1}{k_BT^2}\left(\overline{E^2} - \overline{E}^2\right) = \frac{1}{k_BT^2}\Delta E^2 \quad (6)$$

$$\chi = \frac{1}{k_BT^2}\Delta M^2 \quad (7)$$

The Equivalence with Binary Alloys [9]

We consider an equiatomic binary alloy with *N/2* atoms of type A and *N/2* atoms of type B, each type of atoms being arranged in particular sites for the ordered low temperature phase (sites α for A and β for B). The disordered high temperature phase is obtained when there is an equal number of atoms A (B) in sites β and α. When looking into the order-disorder phase transition in binary alloys, the order parameter will behave exactly as the magnetization for FM/PARA phase transition. For this to be done, we consider the quantity:

$$p_n = P_n^A = \begin{cases} 1, & \text{if the site } n \text{ is occupied by an atom } A \\ 0, & \text{if the site } n \text{ is occupied by an atom } B \end{cases} \quad (8)$$

The fraction of atoms A situated on α and β sublattices are given respectively by:

$$r_A = \frac{1}{N_A}\sum_{n\in\alpha} P_n^A \quad (9)$$

$$w_A = \frac{1}{N_A}\sum_{n\in\beta} P_n^A \quad (10)$$

It is obvious that, $r_A + w_A = 1$. For $T = 0K$, $r_A = 1$ and when T tends to infinity, $r_A = w_A$.

If we consider similar parameters for B (r_B and w_B), taking into account the relation

$N_\alpha = N_\beta = N/2$, we can write:

$$\begin{cases} r_A = r_B = r \\ w_A = w_B = w \end{cases} \quad (11)$$

The order parameter is obtained from these quantities as follows:

$$\varepsilon = \frac{r - w}{r + w} = 2r - 1 \quad (12)$$

- For $T = 0$K , $r = 1$ and $\varepsilon = 1$
- For $0 < T < T_c$, $1/2 < r < 1$ and $0 < \varepsilon < 1$
- For $T > T_c$, $r = 1/2$ and $\varepsilon = 0$

The equivalence with the Ising model is not only at the level of the order parameter, but also at that of the energy of the system. This energy can be written in the form [10]:

$$E = E_0 - \frac{v}{2} \sum_{(i,j)_v} S_i S_j \quad (13)$$

Here, E_0 and v are functions of the interaction energies between pairs of nearest neighbours. $S_i = +1$ if we have a site α occupied by an atom A or a site β by an atom B. $S_i = -1$ if we have a site α occupied by an atom B or a site β by an atom A.

By a suitable choice of the origin of energy, relation (13) is approximately the same as the energy of the Ising model with no external field.

ANTIPHASE PHENOMENA-NUMERICAL SIMULATIONS

Antiphase Phenomena in Crystals

APB in crystals can be due to the presence of partial dislocations [6]. Contrary to the case of classic dislocations, the Burgers vectors of partial dislocations are not proportional to the lattice vectors. From here comes the creation of a band of misplaced atoms called APB. Partial dislocations can be obtained by:

i) A stacking fault [11] arising from any arrangement of atoms different from the ABABAB… (HCP structure) or ABCABC… (FCC structure) arrangement of atoms.

ii) A dissociation of dislocations in some structures like superalloys [11, 12]. Here, a superdislocation (SD) can split into two superpartials (SP) and an APB. But those superpartials can also split into two partials (P) and a stacking fault (SF). We can summarize it with the following diagram :

$$SD \rightarrow SP + APB + SP \rightarrow (P + SF + P) + (APB) + (P + SF + P)$$

Those dislocations split because their energy should take a minimum value. In fact, the energy of a dislocation of Burgers vector $\vec{b}$ is given by $E_{\vec{b}} \approx G\vec{b}^2$ where G is a quantity depending on the shear modulus of the crystal. If this dislocation splits into two partials of Burgers vectors $\vec{b_1}$ and $\vec{b_2}$, we have the relation :

$$E_{\vec{b}} = E_{\vec{b_1}+\vec{b_2}} \approx G\left(\vec{b_1} + \vec{b_2}\right)^2 > G\vec{b_1}^2 + G\vec{b_2}^2 \quad (14)$$

which shows that the energy of the partials is less than that of the classic.

Antiphase in the Ising Model

Here, we have the "Antiphase" and Antiphase Boundaries:

Antiphase: It is a particular phase obtained for some models like the Binary Next-Nearest-Neighbours Ising (BNNNI) and the Anisotropic Next-Nearest-Neighbours Ising (ANNNI). Here, the interaction between next nearest neighbours along a particular direction is taken into consideration. The coupling constant between the nearest neighbours and that between next nearest neighbours should have opposite signs. For some values of the two constants, the Antiphase is obtained. It is neither a FM nor an AFM phase, but an alternatively two up - two down arrangements of spins (See figures 1 and 2).

In the BNNNI [13, 14], the NNN interaction is considered along two directions. The Hamiltonian has the form:

$$H = -J_1 \sum_{\langle i,j\rangle nn} S_{ij} S'_{ij} - J_2 \sum_{\langle i,j\rangle bnnn} S_{ij} S''_{ij}$$

or $$-\frac{H}{k_B T} = K_1 \sum_{\langle i,j\rangle nn} S_{ij} S'_{ij} + K_2 \sum_{\langle i,j\rangle bnnn} S_{ij} S''_{ij} \qquad (15)$$

Where $K_1 = J_1 / k_B T$ and $K_2 = J_2 / k_B T$. K_1 and K_2 have opposite signs.

In the ANNNI model, the NNN interaction is taken only in one direction. The energy deduced from its two dimensional Hamiltonian is given by [15]:

$$E = -\frac{H}{k_B T} = K_1 \sum_{\langle i,j\rangle} S_{i,j} S_{i+1,j} - K_2 \sum_{\langle i,j\rangle} S_{i,j} S_{i+2,j} + K_0 \sum_{\langle i,j\rangle} S_{i,j} S_{i,j+1} \qquad (16)$$

Here, the Antiphase obtained is similar to that of the BNNNI but we make sure the ground state in the y-

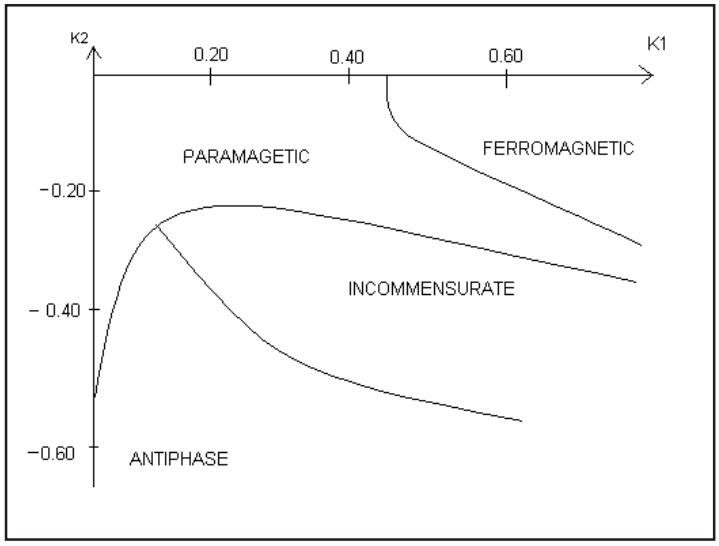

Figure 1:Phase diagram of the Binary Next-Nearest-Neighbours Ising (BNNNI) for $K_1 > 0$ and $K_2 < 0$

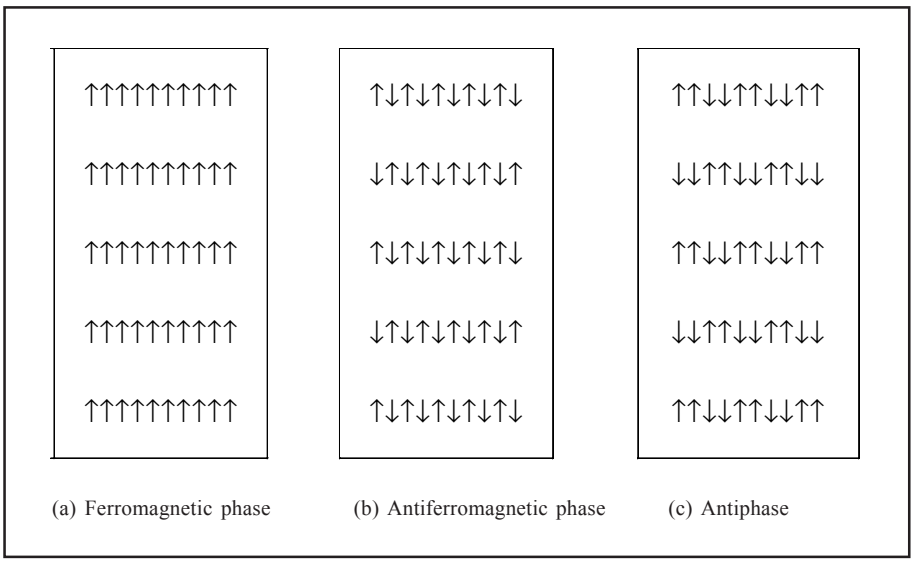

Figure 2:Low temperature phases of the BNNNI model. The antiphase is characterised by an alternatively two up-two down arrangement of spins.

direction is ferromagnetic and the modulation (2,2) runs only for the x-direction.

Antiphase Boundaries: They are obtained by introducing interfaces (to turn over some spins) in FM or AFM arrangement of spins. The process depends on the space dimension. It has been observed that in AFM interaction, periodic boundary conditions introduce FM bonds in square lattices with odd linear size L. Figure 3 refers to $L=5,6,9$ and 10.

By considering periodic boundary conditions, the spin (i,j) should be pointed in the same direction as the spin $(i+L, j+L)$. Here, i and j refer to the spin coordinates respectively in x- and y-directions. The generated lattice has the size $(L+2)^2$, and the spins of the following groups of spins are pointed in the same direction:

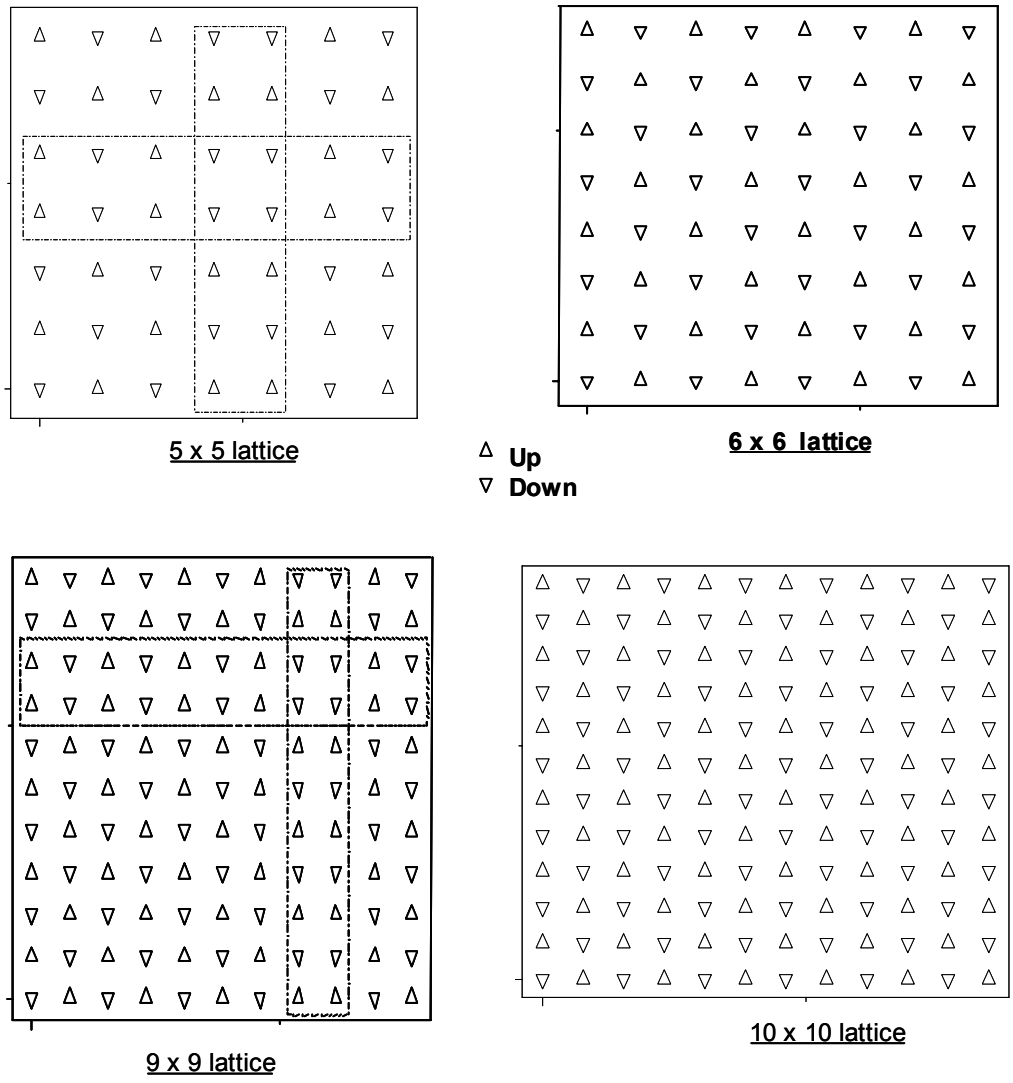

Figure 3: AFM interaction with PBC lead to the creation of APBs in lattices with odd linear size (inside dashed lines). There are no APBs for lattices with even linear size.

(1,1) = (1,L+1) = (L+1,1) = (L+1,L+1)
(1,L) = (1,0) = (L+1,0) = (L+1,L)
(L,1) = (0,1) = (0,L+1) = (L,L+1)
(L,L) = (0,0) = (0,L) = (L,0)

and

(1,j) = (L+1,j); j = 2, L–1.
(L,j) = (0,j); j = 2, L–1.
(i,1) = (i,L+1); i = 2, L–1.
(i,L) = (i,0); i = 2, L–1.

The area made up of spins with FM bonds (up-up or down-down) is called APB. Thus, this situation is similar to what happen in solids, because APB prevents the system from reaching the ground state, by increasing its energy. This is what we have verified by numerical simulations.

Numerical Simulations

The numerical simulations were done with a Monte Carlo code written in Fortran 77. The initial configuration was obtained by using for each spin of the lattice a random number belonging to the interval 0 and 1. If this number is less than 0.5, the spin is up. The spin is down otherwise. We first made sure that PBCs that are responsible for the creation of the APB are considered. The number of Monte Carlo cycles and the number of iterations were set accordingly to the size of the lattice.

The previous configuration of the lattice was taken to be the initial configuration for the next step. At a given temperature, the value of the quantity that is being calculated (energy, magnetization, specific heat) is the mean value over the number of iterations set before. Due to long equilibration at a given temperature and the fact that we have taken small temperature steps, the curves we obtained are very smooth. Several lattice sizes have been considered and sometimes both FM and AFM interactions.

RESULTS

The curves obtained for different lattice sizes and for the same thermodynamic function are similar and lead to the same interpretation. This is the reason why we will not report all of them here. Figure 4 shows the energy versus temperature curves for L=15 and L=16 square lattices, both in FM and AFM interactions.

The energy of the normal ground state is $E_{min} = -2\ (J/k_BT)$. But in 15×15(AFM) lattice, $E_{min} \approx -1.72$. This is not the case for 15×15(FM), 16×16(FM) and 16×16(AFM) lattices for which $E_{\min} = \square 2$. The same behaviour has been observed for 31×31, 32×32, 64×64… lattices.

The curves of the specific heat are represented in figure 5 for15×15 and 16×16 square lattices in AFM interaction. It is easily seen that the phase transition occurs approximately at the temperature $T_c = 2.26(J/k_B)$ for both odd and even *L*. Nevertheless, for even *L*, the curve has a clear peak, and that is not the case for odd *L* where we observe a subsidence.

It is known that there should be no magnetization when the system is in PARA or AFM state. This has been confirmed by the curves obtained (fig. 6). However, if we change the scale, we observe a weak fluctuating magnetization around 0 at low temperature for lattices with odd *L*, whereas for even *L* the magnetization is really 0 when the temperature tends to 0 (fig. 7). This is due to APB that introduces a symmetry breaking in the spins arrangement. This difference in the behaviour of the magnetization is significant only at the macroscopic scale.

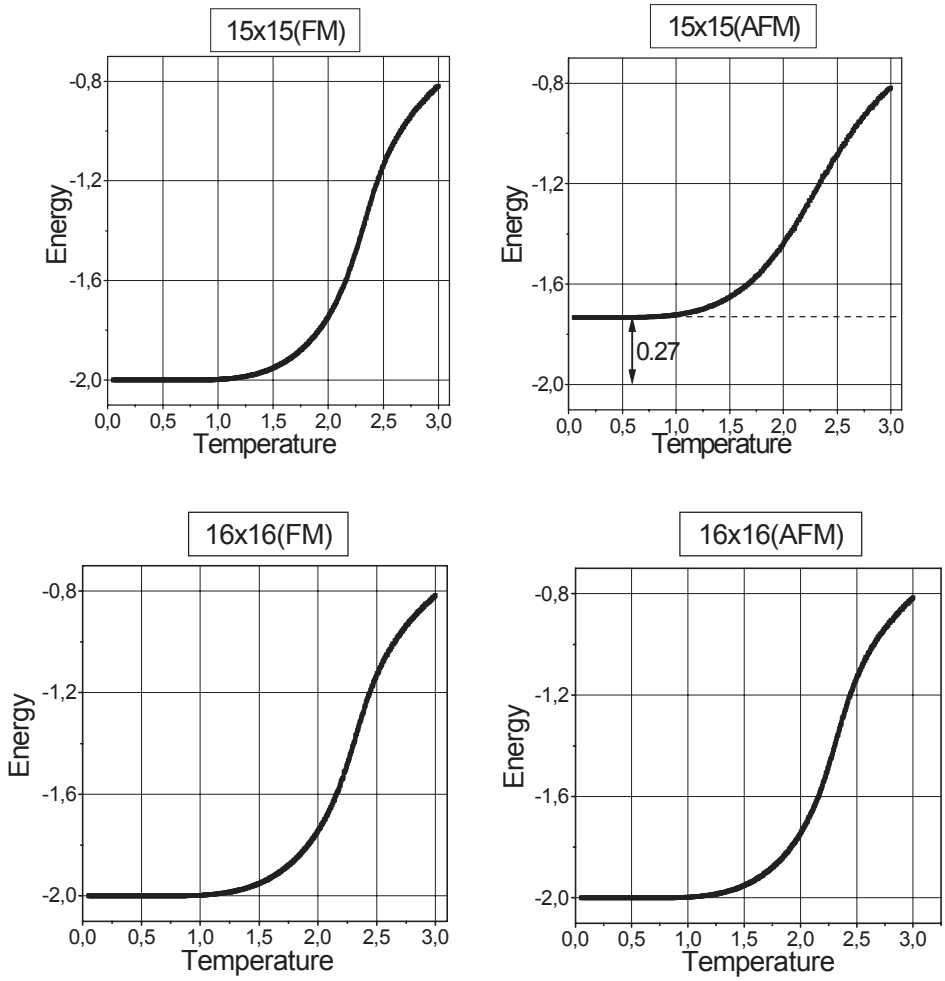

Figure 4: *L=15* and *L=16* in Ferromagnetic (FM) and Antiferromagnetic (AFM) interaction. The energy gap (0.27) observed in 15×15(AFM) lattice as the temperature tends to 0 K is due to the presence of APBs

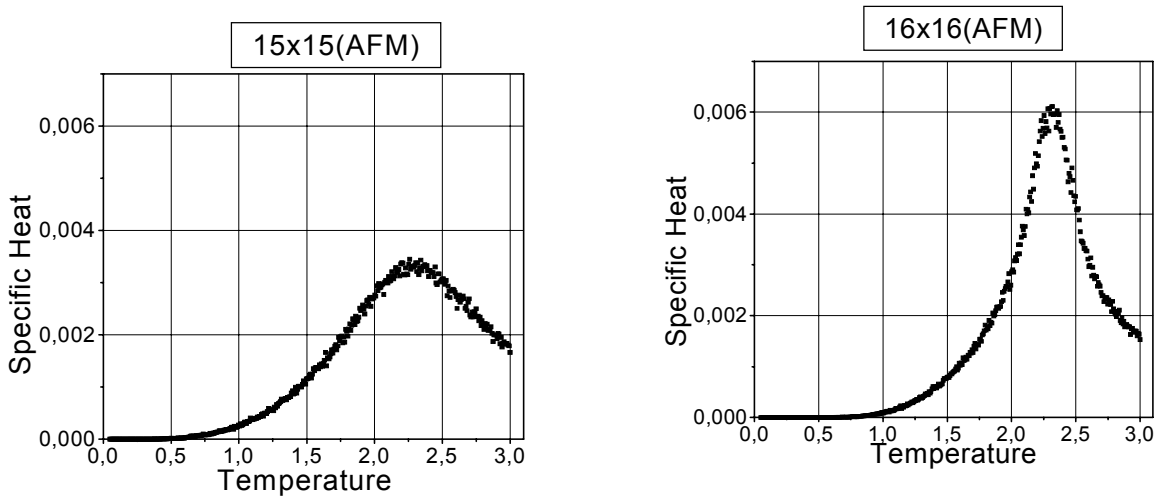

Figure 5: Specific heat of 15×15(AFM) and 16×16(AFM) lattices. The AFM/PARA phase transition is clearly observed for 16×16(AFM) lattice

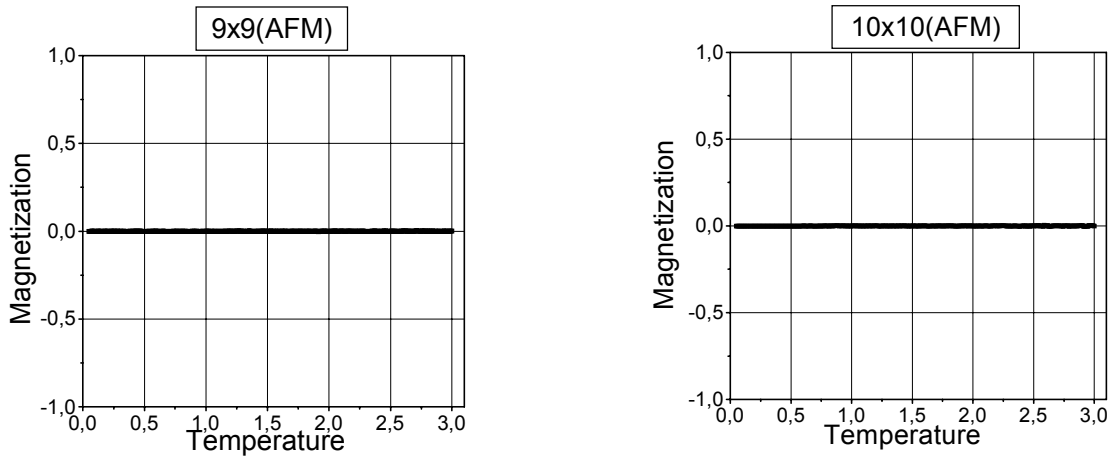

Figure 6: 9×9(AFM) and 10×10(AFM) lattices. The magnetization has a zero value before and after the phase transition

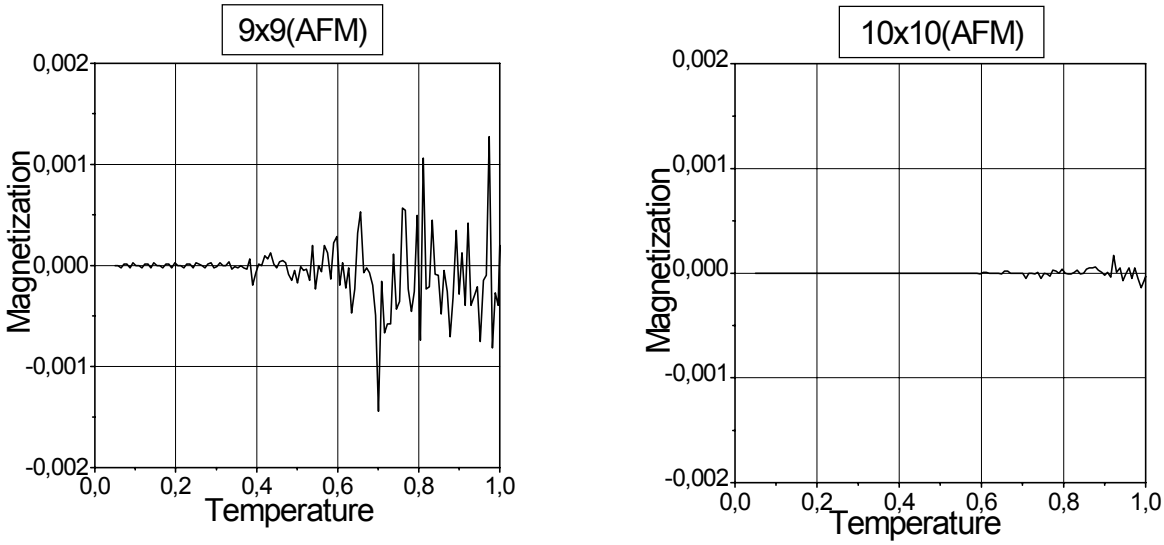

Figure 7:Fluctuation of the magnetization around zero even in AFM phase for 9×9(AFM) lattice. For odd linear size lattices, fluctuations are more important because of the PBCs that introduce some FM interactions

DISCUSSIONS

From the curves obtained, it is observed that the energy of the fundamental FM state is –2 (in unit of $|J|/k_B T$) for odd and even *L* lattices. This value coincides with theoretical predictions (previous sections). We have the same value for even *L* lattices in AFM interaction, but for odd *L* lattices, there is an energy gap which is due to APB arising from PBCs. Here, the real fundamental state is not observed, since the interaction energies between spins do not have their minimum values. In fact, the spins of the APB are parallel whereas they should be antiparallel: this energy gap is said to be contained in the APB. Numerical evaluation of the Ni_3Al APB energy has been done using the so called λ-integration method [16].

Let us evaluate the excess of energy due to APB. Since the total size of the generated lattice is not taken into consideration during measurements, our calculation should involve only the spins contained in the area of size L^2, but not $(L+2)^2$. It is observed that in this area, 10 FM bonds are introduced in 5×5 lattice, 14 in 7×7, 22 in 11×11 … Thus, for L×L lattice, (2*L*) FM bonds are introduced.

In AFM ($J<0$) low temperature phase, the interaction energy of two neighbouring spins is $E_{AFM} = -JS_iS_j = J$ (S_iS_j = -1). If the interaction between them becomes FM, the energy is $E_{FM} = -JS_iS_j = -J$ (S_iS_j=+1), *J* being the same. The difference of energy is therefore:

$$\Delta E = E_{FM} - E_{AFM} = -J - (J) = -2J = 2|J| \quad (17)$$

Thus, at a given temperature, the introduction of one FM bond in the AFM lattice increases its energy by $2|J|$. If we denote ε_0 the energy of the lattice when all bonds are AFM and ε its energy when (2*L*) FM bonds are introduced, we have the relation:

$$\varepsilon = \varepsilon_0 + [2L]\left(2|J|\right) = \varepsilon_0 + 4|J|(L) \quad (18)$$

or $\frac{\varepsilon}{k_BTL^2} = \frac{\varepsilon_0}{k_BTL^2} + \frac{4|J|}{k_BTL^2}(L)$ which is the energy per spin. Let us denote $E = \frac{\varepsilon}{k_BTL^2}$ and $E_0 = \frac{\varepsilon_0}{k_BTL^2} = -2\left(\frac{|J|}{k_BT}\right)$. Then we can write:

$$E = E_0 + \frac{4|J|}{k_BT}\left(\frac{L}{L^2}\right) = \left(4\left(\frac{L}{L^2}\right) - 2\right)\left(\frac{|J|}{k_BT}\right) = \left(\frac{4}{L} - 2\right)\left(\frac{|J|}{k_BT}\right) \quad (19)$$

Thus, in unit of $|J|/k_B T$, the energy per spin of the lattice at low temperature is:

$$E = \frac{4}{L} - 2 \quad (20)$$

L being an odd number.

The energies evaluated from this formula are shown in table 1 (E_{theo}) along with the values obtained from simulations (E_{sim}). One can observe that results of simulations are almost the same as those predicted by the theory. Thus, the gap of the energy can be written as:

$$\Delta E = E - E_0 = \frac{4}{L} \quad (21)$$

Table1: Simulated (E_{sim}) and theoretical (E_{theo}) values of energy per spin at low temperature $\left(T \approx 0.05\ (|J|/k_B)\right)$, for odd linear size lattices *L*.

L	E_{sim}	E_{theo}
9	-1.55555560	-1.55555555
31	-1.87164816	-1.87096774
63	-1.93650794	-1.93650793
127	-1.96850394	-1.96850393
191	-1.97905759	-1.97905759
209	-1.97685739	-1.98086124
259	-1.98455598	-1.98455598
289	-1.98615917	-1.98615917
369	-1.98915989	-1.98915989
429	-1.99067599	-1.99067599
469	-1.99147122	-1.99147121
489	-1.99182004	-1.99182004

Relation (21) shows that an increase in the value of *L* is accompanied by a decrease in ΔE. This is exactly what we observed in the curves obtained from our simulations. This situation can be compared to what happen in alloys where it is shown that the APBs energy is proportional to

the inverse of its width [1]. More precisely, the gap of energy decreases because as the size of the lattice is high, the APB becomes longer, but the fraction of spin involved in the boundary becomes weak. The fraction *P(L)* of the *4(L-1)* spins involved in the APB in the area of size L^2 is:

$$P(L) = \frac{4(L-1)}{L^2} \tag{22}$$

It is easily shown that:

$$\frac{dP(L)}{dL} = -\frac{4(L-2)}{L^3} \tag{23}$$

Since *L>2*, $\frac{dP(L)}{dL} < 0$. Thus, *P(L)* is a decreasing function of *L*. If the size of the lattice is high, the energy of the boundary is relatively small.

On the other hand it is observed in the above figures that for all lattices whatever the size and the interaction, the energy at high temperature is – 0.8 (in unit of $|J|/k_B T$) which shows that the effect of APB at this range of temperature (paramagnetic phase) is not pointed out. This is a general behaviour attributed to entropic effects at high temperatures. This is also confirmed by the magnetization which presents a significant difference at low temperature but not as the temperature increases, as we can observe in figure 7.

CONCLUSION AND PERSPECTIVES

Using the Monte Carlo simulations applied to the two dimensional Ising spin model, we showed that in anti ferromagnetic square lattices with odd linear size *L*, the periodic boundaries conditions create and energy gap that prevents the system from reaching the ground state energy. We have established that this energy gap is proportional to the inverse of the linear size characteristic *L* of the system. For this result to be more expressive, the energy gap has to be related to a lattice parameter in real materials. This is one of our future preoccupations.

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