Two dimensional Ising model with Einstein site phonons

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(Dated: April 16, 2019)

We consider a simple Ising magnetic model in two dimensions with Einstein site phonons and study it using Monte Carlo simulations that take into account both degrees of freedom simultaneously.

In every real magnetic material there is an interplay between the magnetic and elastic degrees of freedom. While in many cases this is of no consequence for the magnetic order, and can be neglected, there are a growing number of cases where this interplay is key to understanding the ground state and excitations of magnetic materials. Starting with the theoretical prediction of the so-called ‘spin-Peierls’ effect, a progressive spin-lattice dimerization occurring at low temperatures, observed experimentally for the first time in CuGeO$_2$ [1], there has been a rapidly growing literature that addresses this issue both from theoretical and experimental perspectives.

Theoretical models have considered classical Ising and Heisenberg models coupled with global Debye distortions (e.g. Ref. 3 or Ref. 10), unconstrained (the bond model of Ref. 6) and Einstein site phonons (e.g. Ref. 8 or Ref. 9) which are a good approximation for systems dominated by optical phonons. Treating both degrees of freedom simultaneously can be a daunting task. Some simulations exist in the literature [3-10], but the usual method is to perform a Gaussian integral over the set of displacement coordinates in the partition function. The phonons are then integrated out to obtain an effective spin Hamiltonian which redresses the exchange constants and can introduce additional interaction terms (see e.g. Ref. 8). Analytical work, or simulations, are then performed on the effective system.

The two-dimensional Ising model is probably the simplest magnetic model to show a non-trivial phase transition, and is among the most studied models. Surprisingly there is no work in the literature that describes the case of the 2D-Ising model under Einstein distortions. In this work we do a full Monte Carlo simulation, treating simultaneously spin and elastic degrees of freedom, of the classical Ising model on the square and kagomé lattices. Following Ref. 8 we consider Einstein distortions and a linear coupling between both degrees of freedom. The model and the Monte Carlo algorithm used for the simulations and the consistency checks performed on our system are discussed in Sec. II. A conception usually found in the literature is that distortions are important only in frustrated systems and that their main effect is to help ordering by relief of frustration. Instead, we find that in the unfrustrated square lattice (Sec. IIIA) this coupling weakens the magnetic ordering transition into the fully polarised state. Upon increase above a critical value the coupling leads to a structural distortion simultaneous with ordering into a different magnetic state, which we label a checkerboard phase, or CB. This CB phase is a zero-magnetisation state, composed of ferromagnetic clusters ordered anti-ferromagnetically with respect to each other. In the frustrated kagomé case (Sec. IIIB) we find above a critical coupling an ordered state which shares many similarities with the CB phase.

II. MODEL AND METHODS

For our study we use a simple model that takes into account the coupling between magnetic and elastic degrees of freedom the so-called Einstein site phonon spin model. In this model, the sites have independent displacements given by a set of independent harmonic oscillators. Here one is assuming that the most important lattice distortion contribution is coming from optical phonons. This is a reasonable assumption given that in real materials the active magnetic lattice is usually a sub-lattice of a more complex crystal structure (e.g. the pyrochlore Dy lattice in Dy$_2$Ti$_2$O$_7$). The Hamiltonian is then given by

$$\mathcal{H}/|J_0| = \sum_{<i,j>} J(r_{ij}) S_i S_j + K_e \sum_i |\mathbf{u}_i|^2. \tag{1}$$

Here $|J_0|$ gives the energy scale, $J(r_{ij})$ is the exchange constant in units of $J_0$ that depends on the relative position of the sites $i$ and $j$, $S_i$ are Ising variables and the sum $\langle i, j \rangle$ is over nearest neighbors only. The $\mathbf{u}_i$ are the dimensionless displacements for each site $i$ in units of the the undistorted nearest neighbours distance $a$ and $K_e$ is a dimensionless elastic constant. If we consider
the displacements to be sufficiently small compared with
the lattice parameter (|u| ≪ a) then it is reasonable to
expand J_{ij} to a linear dependence on the relative site
positions r_{ij}

\[ J(r_{ij}) = \text{sgn}(J_0)(1 - \alpha(r_{ij} - 1)), \]

(2)

where \( \alpha \) is a dimensionless coupling constant. We will
use \( \alpha \) as a control parameter to measure the degree of
 coupling to lattice distortions.

To simulate the elastic distortions we consider polar
coordinates, \( \theta \) is treated like a clock model of 360 equally
spaced angles and the displacement, \( \rho \) is chosen randomly
in a distribution from 0 to a temperature dependent maximum \( \delta_{\text{max}}(T) \). The use of the latter has no impact on
the results obtained from the simulation, it is introduced
merely as a way to optimise the speed of the simulations
by avoiding the proposal of extremely unlikely moves
at low temperatures. To determine \( \delta_{\text{max}}(T) \) we simu-
late a spin-less lattice with a large \( \delta_{\text{max}} \) and calculate a
histogram of the displacements at several temperatures.
From each of these we choose a \( \delta_{\text{max}}(T) \) such that it in-
cludes 80% of the histogram. We then fit a power law
to these points and use the fitted function in the simu-
lations. The function that fits best has, as expected, a
square root dependence in \( T/J_0 \). A spin-less simulation
of a square lattice using this algorithm gives the correct
specific heat \( (C_v = 1) \) and the correct temperature de-
pendence for the mean square displacement \( (\langle u^2 \rangle \propto T) \).

In our Monte Carlo simulation we treat simultane-
ously the magnetic and elastic degrees of freedom using a Born-
Oppenheimer (BO) approximation, that is, by assuming
that the relaxation times of the magnetic degrees are
much shorter than the elastic. Each step of the simu-
lation is split into elastic and magnetic moves. The BO
approximation translates into the fact that each elastic
move is done with a relaxed magnetic configuration. The
algorithm proceeds as follows:

We do \( P \) elastic Monte Carlo steps (MCS), each of
which consists of the following:

1. Choose a random site.

2. Propose a move by picking at random an angle and
   a displacement (from 0 to \( \delta_{\text{max}} \)).

3. Calculate the exchange constants for the proposed
   spacial configuration.

4. Calculate the total energy of the system (magneti-
   c+elastic) and accept or reject the move ac-
   cording to Metropolis.

5. Make \( Q \) magnetic moves, each move consists of:
   (a) Flip one spin at random
   (b) Calculate the change in magnetic energy
   (c) Accept or reject according to Metropolis
   (d) Repeat (a) to (c) until each spin has been
       chosen at least once on average.

6. Repeat 1. to 5. until each site has been chosen at
   least once on average.

We have checked that our results are independent of
the precise choice of the ratio \( P/Q \) by running different
simulations on lattices with \( N \) sites with \( Q \) varying from
1 to 300, that is, the number of moves for each \( Q \) be-
ing from \( N \) to \( 300N \) times those for \( P \). We have
used square lattices with \( L \) from 4 to 24 and typically
with \( P = 10^7 \) MCS. Quantities are averaged over time
after a waiting period of \( P = 50000 \) MCS to allow for
equilibration (see 22). The figures in this paper are all for
\( L = 16 \).

The energy scales for magnetic and elastic degrees of
freedom can be characterised by the critical temperature
of the decoupled Ising system, \( T^*_0 \), and the melting
temperature, \( T^* \). The latter can be defined in our system by
means of the Lindemann criterion in two dimensions
(\( \sqrt{(u^2)} \approx 0.1 \)), and the former can be determined by sim-
ulating the decoupled magnetic system. Using equipar-
tition one gets \( T^* \approx |J_0| K_c/200 \). In order to work
in the limit \( |v| \ll 1 \) one must choose \( K_c \) such that
\( T^* \approx 1 \). For the simulations of this work we have
chosen \( K_c = 7200 \) which means \( T^* \approx 15 \).

A simple checkup of the simulation algorithm is to
compare the results obtained for \( \alpha = 0 \), that is, no cou-
pling between elastic and magnetic degrees of freedom
with the results obtained from a Metropolis simulation
of an Ising model on a fixed lattice. Figure 1 shows such a
comparison for the specific heat of a \( L = 16 \) square
lattice. The orange curve corresponds to the static Ising
system. As expected, the decoupled elastic system is sim-
ply a sum of the elastic contribution \( (C_v^\text{el} = 1) \) and the
magnetic contribution which is identical to the static sys-

FIG. 1. Comparison between the specific heat of a decoupled
elastic system (blue line, left axis) and a static Ising system
(orange line, right axis). As expected the specific heat of the
former is a simple sum of the elastic contribution \( (C_v^\text{el} = 1) \)
and the magnetic Ising part (the right axis is shifted accord-
ingly in the plot).
FIG. 2. Specific heat, $C_v$, (upper panel) and magnetisation, $M$, (lower panel) as a function of temperature for a series of fixed values of $\alpha$ below $\alpha_c$ (see legend). The ferromagnetic transition progressively moves to lower temperatures as $\alpha$ is increased until it eventually vanishes at $\alpha_c$. The lower panel shows a snapshot of the ordered state.

III. RESULTS

A. Square lattice

In what follows we will describe the results obtained for ferromagnetic interactions. The antiferromagnetic case can be obtained by the usual mapping $S_A \rightarrow -S_A$, $S_B \rightarrow S_B$, where $A$ and $B$ are the two disjoint sublattices of the square lattice. We find it useful in terms of presenting the results to separate the discussion for values of $\alpha$ above and below the critical value $\alpha_c$ at which the ordering transition vanishes.

1. $\alpha < \alpha_c$: the ferromagnetic transition

Figure 2 shows the specific heat and magnetisation (the order parameter for the FM transition) as a function of temperature as obtained from our simulations for a series of runs with increasing values of the coupling parameter $\alpha$. The data shows that the ferromagnetic (FM) transition moves towards lower temperatures as $\alpha$ is increased. As expected, the peak in the specific heat (upper panel) becomes sharper as the critical temperature is reduced, and so does the step towards saturation in the magnetisation (lower panel). If $\alpha$ is further increased, the FM transition temperature sinks towards zero at $\alpha_c = 60$ (for this given value of $K_c$). A calculation of $\alpha_c$, which becomes clear once the ordered state for high values of $\alpha$ is known, is given in the appendix.

Figure 3 shows the mean value of the displacement, $\langle u \rangle$, as a function of temperature for different $\alpha$ below $\alpha_c$. In the absence of any coupling ($\alpha = 0$) the curve follows the expected $\sqrt{T}$ behaviour (dotted line). For coupled systems the displacement follows the same curve at low temperatures and jumps up at the magnetic transition and follows a $\sqrt{T}$ dependence with an increasingly higher pre-factor (see text). The inset shows $\langle J_{ij} \rangle$ as a function of $T$ for the same values of $\alpha$.
netisation domains. As usual in any Ising transition, the systems start splitting into domains of opposite magnetisation, but the unusual mechanism in this case is that the antiferromagnetic walls between domains are accompanied by distortions that change the sign of the exchange constant and thus render them stable. This mechanism favours the existence of domains of opposite magnetisation and thus conspires against the FM order. To ascertain the existence of these two mechanisms beyond the mere inspection of snapshots we constructed a histogram of $J_{ij}$ as a function of temperature. The upper panel of figure 4 shows such a histogram for $\alpha/\alpha_c = 5/6$ using a data window in $J_{ij}/|J_0|$ between -20 and 20, with a binning of 0.002, and collecting data over $P = 10^7$ MCS. The distribution resembles a Gaussian centred around $J_{ij}/|J_0| = -1$ that increases its half-

maximum width as the temperature is increased. However, a closer inspection reveals that the distribution is slightly skewed towards positive $J_{ij}$. A quantitative way of seeing this is by comparing the value of $J_{ij}$ at the maximum with $\langle J_{ij} \rangle$, which should coincide for a symmetric distribution. This is shown in figure 5 for $\alpha/\alpha_c = 5/6$. Below the FM transition, $T_c(5/6)/|J_0| = 0.75$, both the maximum and the mean value coincide, but at $T_c$ there is a jump after which the maximum lies at a considerably lower value than the mean. This is evidence of the stabilisation of positive values of $J_{ij}$ around the domain borders. This type of mechanism is particular to the Ising case and should be absent in a Heisenberg system. Indeed, numerical studies of a coupled spin-lattice system with Heisenberg-like spins show that in this case the transition is only marginally affected by the coupling to vibrations.

2. $\alpha > \alpha_c$: The checkerboard transition

If the coupling parameter $\alpha$ continues to be increased a new ordered state develops at low temperatures. The upper panel of figure 6 shows the specific heat above $\alpha_c$. As seen in the figure, there is a sharp peak in the specific heat for $\alpha > \alpha_c$ that increases in temperature as $\alpha$ is increased. A snapshot of the ordered state that is found at low temperatures in this case is shown on the upper part of figure 7. This is a zero-magnetisation state where the lattice breaks into clusters of four spins with equal orientation, ordered anti-ferromagnetically with respect to each other. We have shaded the clusters in red and

![FIG. 4. Histograms for the pair exchange constants, $J_{ij}$ at different temperatures. In the upper panel for $\alpha < \alpha_c$, and in the lower panel for $\alpha > \alpha_c$. Below $\alpha_c$, the distribution resembles a Gaussian centred around -1, but closer inspection shows it is skewed to the right at temperatures close to $T_c/|J_0| = 0.75$ (see text for details). Above $\alpha_c$, it is a bimodal distribution with two clearly defined FM and AFM peaks that merge as the temperature is raised.](image-url)
blue to emphasise the checkerboard nature of this state. The pair exchange interactions \( \langle J_{ij} \rangle \) are shown as circles in the midpoint between bonds, coloured according to the scale shown in the right. The distortions are exaggerated tenfold in the picture for visual clarity.

This state (which we will call CB for short) is a sort of dimerisation in two-dimensions: the spins in the clusters are closer to each other (thus enhancing ferromagnetic interactions) and further apart from their neighbours in the other cluster (thus turning this interaction antiferromagnetic). It is straightforward to notice that the \( J_{ij} \) show a bimodal \( FM - AFM \) distribution, which is readily seen in the histograms for \( \alpha > \alpha_c \). An example of these is shown in the lower panel of figure 4, for \( \alpha/\alpha_c = 7/6 \). Below the transition temperature \( (T_c(7/6) \approx 0.7) \) there are two separate peaks that evolve into two sharply defined identical peaks at low temperatures at \(-4|J_0|\) and \(2|J_0|\) (averaging \( -|J_0| \)).

To characterise this transition it is useful to calculate an order parameter. We use a unit-cell like the one shown in figure 7. We define an index \( j \) that runs over all squares in the lattice such that it counts as odd and even the squares marked with 1 and 2 respectively in the picture, and an index \( a \) that runs over the spins in the squares. There are four possible degeneracies of the ground state (plus time reversal), corresponding to where the coloured squares are set in the unit cell. We then define an order parameter \( \Phi \) that is the sum over the four possibilities, \( \Phi = 1/N \sum_{m=0}^4 (-1)^m |\Phi_m| \), where

\[
\Phi_m = \sum_{j=1}^{N/4} \sum_{a=1}^4 (-1)^j e^{i\phi_a^m} \sigma_a^j.
\]

Here \( \sigma_a^j \) are Ising-spin variables that can take the values \( \pm 1 \), \( N \) is the total number of spins, and the \( \phi_a^m \) are the phase factors for the spin that take into account the four possible degeneracies: \( \phi_1 = \pi(0, 0, 0, 0) \), \( \phi_2 = \pi(1, 0, 1, 0) \), \( \phi_3 = \pi(1, 1, 0, 0) \), \( \phi_4 = \pi(1, 0, 0, 1) \).

The lower panel of figure 6 shows the evolution of the order parameter \( \phi \) as a function of temperature for different fixed values of \( \alpha \) (indicated in the figure). As expected, there is a jump in \( \phi \) that coincides with the peak in the specific heat. The jump is sharp for \( \alpha \) close to \( \alpha_c \) and softens as \( \alpha \) increases. An inspection of the mean value of the displacement \( \langle u \rangle \), figure 8, shows that the magnetic ordering corresponds with a jump in \( \langle u \rangle \), i.e., there is a simultaneous magnetic and structural transition. This jump in \( \langle u \rangle \) in turn relates with the separation of the peaks in the histogram of \( J_{ij} \) that we have discussed earlier. Figure 8 also shows that \( \langle u \rangle \) remains non-zero as \( T \to 0 \) above \( \alpha_c \). It is straightforward to calculate \( \langle u(T = 0) \rangle \) as the minimum from the two possible ground states (\( FM \) and \( CB \)). The expression, calculated in the appendix, is simply

\[
u_{\min}(\alpha) = \begin{cases} 0 & \text{if } \alpha \leq \alpha_c, \\ \frac{\sqrt{2} \alpha_c}{\sqrt{1 - \alpha_c^2}} & \text{if } \alpha > \alpha_c. \end{cases}
\]

This is shown as a red line in figure 9 together with the values obtained from the simulations (open circles). As it can be seen there, there is a sharp step in \( \langle u(T = 0) \rangle \) at \( \alpha_c \) corresponding to a structural transition that lowers the lattice symmetry.

When \( \alpha \) is close to \( \alpha_c \) the distortions are still small and there are states with long-range order that have energies comparable with the ground-state. It is very frequent that for these values of \( \alpha \) the simulated system will remain at a local minima. One such possible state is pictured in the bottom part of figure 7. This is still a dimerised state, with pairs of equally-pointing spins ordered anti-ferromagnetically, but it corresponds to a shift in the phase (by \( a \)) in consequent horizontal rows. In this state the \( J_{ij} \) order in stripes, and so do the spins (shaded red and blue). In all other respects it shares the characteristics of the ground-state (bimodal distribution, jump in the distortion, etc.) If the distortion is small, this costs very little energy, but it becomes progressively disfavoured as \( \langle u \rangle \) increases. The snapshot corresponds to a
small distortion configuration, but, as we mentioned before, the distortion in the figure has been multiplied by an order of magnitude to make it apparent.

Similar phases are known to be brought about by coupling to lattice distortions in a different context. This is the case of the phonon-induced phases found in the Holstein-Hubbard model. This is a model of a correlated electron system where electron-phonon interactions with Einstein phonons are considered in addition to electron-electron interactions. Contrary to our case, this model treats phonons quantum mechanically and has a coupling to elastic degrees of freedom that is odd in nature, since it was originally conceived for a molecular crystal. For large values of the coupling strength, a bipo-

FIG. 7. Two snapshots of configurations for $\alpha > \alpha_c$. The upper panel shows an example of one of the possible checkerboard states. Here the lattice dimerises into square clusters of equal spin orientation aligned anti-ferromagnetically with respect to each other. The dotted line shows the unit cell. The coloured circles correspond to the values of $\langle J_{ij} \rangle$ in the bond, and are coloured according to the scale on the right. The lower panel shows a stripped phase. This is a low temperature excitation of the CB phase that takes place for values of $\alpha$ close to $\alpha_c$. For visual clarity, in both cases the distortions have been exaggerated tenfold.

FIG. 8. Mean value of the displacement, $\langle u \rangle$, as a function of temperature for different $\alpha$ above $\alpha_c$. The transition into the CB phase is marked by a jump in $\langle u \rangle$ which then intercepts $T = 0$ at a non-zero value. This is the consequence of a structural transition simultaneous with the magnetic one. The inset shows the mean value of the exchange constant.

FIG. 9. Distortion at $T = 0$ as a function of the coupling parameter, $\alpha$. The blue circles correspond to the values obtained from the simulation, and the red line to those predicted by eq. 4. The sharp step at $\alpha_c = 60$ marks the structural transition.

laronic insulator emerges that is reminiscent of the CB phase found here.

3. $T - \alpha$ phase diagram

The $T$-$\alpha$ phase diagram of this system is a sort of summary of the results discussed up to this point. Figure 10 shows the $T$-$\alpha$ phase diagram as obtained from the
FIG. 10. The $T-\alpha$ phase diagram for the FM Ising model on a square lattice obtained from the simulations. The transitions separate a high temperature paramagnet (PM) from the two ground states: the ferromagnet (FM) and the checkerboard (CB). The single line marks a second-order phase transition while the double line marks first-order. The circles, taken from the position of the peak in the specific heat, show some of the data points used to construct the phase diagram.

Simulations. The circles in the figure correspond to the position of the peak in the specific heat.

In the absence of any coupling ($\alpha = 0$) we find the Ising transition from the high temperature paramagnet (PM) into the ferromagnetically ordered state (FM). This second order transition decreases in temperature as $\alpha$ is increased until it sinks to $T = 0$ at $\alpha_c$. When the coupling is increased beyond this point a new ground state emerges, the checkerboard (CB), which is a combination of anti-ferromagnetically ordered ferromagnetic clusters. The CB transition is simultaneous with a structural transition that decreases the symmetry of the lattice.

As we mentioned, the transition below $\alpha_c$ is the expected second order transition in the Ising universality class. This is not the case above $\alpha_c$. The simultaneous occurrence of the magnetic and structural transitions alters the nature of the transition which seems to be first order in the range $1.0 \leq \alpha/\alpha_c \lesssim 1.3$, as determined from the behaviour of the Binder cumulant (not shown)\textsuperscript{30,31}. Some properties show hysteresis in this region when sweeping the temperature up and down. The exact mechanism that determines the range of existence of this first order region is matter of future investigation.

B. Kagomé lattice

We have applied this same simulation algorithm and data analysis to the case of the Ising model on the Kagomé lattice. For the $FM$ case the results follow closely those of the square lattice. In the $AFM$ case, which is frustrated, the systems remains disordered up to a critical value of $\alpha$ above which the frustration is lifted through a simultaneous structural and magnetic transition into the kagomé $CB$ phase (see figure 11). The kagomé $CB$, pictured in figure 12, can also be understood as a dimerisation along the three different axes of the lattice (pictured as ovals of different shades). However, the distribution of the $J_{ij}$ is slightly different, since it is now tri-modal, with two different $FM$ exchange constants corresponding to triangular and hexagonal $FM$ clusters, pictured in the figure in red and blue respectively, which are oriented antiferromagnetically with respect to each other. This is also a zero magnetisation state, since the number of triangles is twice the number of hexagons.

IV. CONCLUSIONS

In this work we have studied the simple classical two-dimensional Ising model on a square an on a kagomé lattice with Einstein distortions. We have performed Monte Carlo simulations of the linearly coupled system taking into account simultaneously both degrees of freedom. In both the unfrustrated square lattice and the frustrated kagomé lattice we find that when the coupling is increased above a critical value the system has a structural transition – a dimerisation along the lattice axes. This occurs simultaneously with magnetic ordering into a clustered state with zero magnetisation, composed of squares in the square lattice, and triangular and hexagonal $FM$
to the appearance of a bimodal distribution of exchange constants in the square lattice, one intra-cluster FM and one inter-cluster AFM, and a trimodal distribution in the kagomé case: two FM interactions (intra-triangles and intra-hexagons) and an AFM interaction inter-cluster. In the unfrustrated case we show that the coupling to the elastic degrees of freedom gradually weakens the transition, through a mechanism whereby domain formation is gradually stabilised by distortions. In the square lattice we identified low-energy excitations consisting of stripes of zigzagging spins. The analysis of the phase diagram shows that the transition into the ordered state is not always second order, but further work is needed to identify the exact boundaries and the mechanisms that are responsible for this.

The main aim of this work was to study one of the simplest possible models with magneto-elastic coupling, and hence the choice of the Ising model on two-dimensions with linear coupling between $J$ and $u$. It can still be questioned whether such a simple model would have any remit of applicability. Detailed descriptions of the dependence $J(u)$ in real materials are scarce. References 32 and 33 provide a careful discussion of the dependence of the magnetic coupling constants of the compound CuGeO$_3$ with respect to lattice distortions. The main magnetic interaction in this case is given by super-exchange paths, but if one makes a simple geometrical model to translate variations in the angle of the mediated pathway into relative displacement between the two magnetic sites, one finds that for the parameters of CuGeO$_3$ displacements in $u_{ij}$ of the order of 3% are well described by a linear dependence of $J(u)$ with a coupling constant that varies from 10 to 90 depending on the value chosen for the undistorted angle, i.e. for $\alpha/\alpha_c$ between 0.16 and 1.5 in the simple Ising model presented here.

ACKNOWLEDGMENTS

We are grateful to R. A. Borzi for discussions an a careful read of the manuscript. This work was supported by CONICET (Argentina), and ANPCYT (Argentina) via grant PICT-2013-2004.

We start by calculating the energy in the CB configuration. Fig. 13 shows a schematic view of the cell used for this calculation.

Taking the assumption that at $T = 0$ $\vec{u}_i$ has identical projections along $x$ and $y$ and one gets

$$\rho_{ij}^{1,2} = 1 + 2 \frac{u}{\sqrt{2}}, \quad (A.1)$$

where $u \equiv u_i = |\vec{u}_i|$. The value of the two exchange constants is then given by

$$J_{1,2} = J_0[1 - \alpha \frac{2 u}{\sqrt{2}} - 1)] = J_0(1 \pm \alpha \sqrt{2} u), \quad (A.2)$$

where we have used that $S_i S_j = \pm 1$ for 1 and 2 respectively.

Thus, the energy per spin of the given unit cell (fig. 13), is given by

$$\varepsilon_{CB}^\text{min} = \varepsilon_{CB}(u_{\text{min}}) = -4 \frac{\alpha^2}{K_{el}} |J_0|. \quad (A.5)$$

On the other hand, the energy of the FM phase is trivially

$$\varepsilon_{\text{FM}}^\text{min} = \frac{E_{\text{FM}}^\text{min}}{N} = -2 |J_0|. \quad (A.6)$$

By equating eqs. A.5 and A.6 one obtains

$$\alpha_c = \sqrt{\frac{K_{el}}{J_0^2}},$$

which gives $\alpha_c = 60$ for the parameters used in this work. This is in good agreement with the value determined by the MC simulations.

It is probably worth noticing that, were the sign of $S_i S_j$ in $J_2$ not be subject to inversion, then $J_1 + J_2 = 2 J_0$, which means that with a linear $J_{ij}$ no deformation would be stable since there would no longer be any gain in the magnetic part of the energy.