Polymerization in a ferromagnetic spin model with threshold

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We propose a spin model with a new kind of ferromagnetic interaction, which may be called *ferromagnetic coupling with threshold*. In this model the contribution of a given spin to the total energy has only two possible values and depends on the number of parallel spins among its nearest and next to nearest neighbors. By mapping the model onto the Ising version of the isotropic eight-vertex model, we obtain some evidence of a low temperature phase made of alternate parallel plus and minus polymers, in which the spin is aligned with the majority of its neighbors. [S1063-651X(96)00808-2]

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I. INTRODUCTION

Ising-like spin systems are much studied statistical models which have a surprising richness of critical behavior (see, e.g. [1]). The axial next nearest neighbor Ising (ANNNI) model is the simplest model which describes modulated structures; experimental evidence for such phases is provided by binary alloys (see, e.g., [2] and [3]). Modulated ordering in the ANNNI model is the effect of the competition between ferromagnetic couplings (between nearest neighbor spins) and antiferromagnetic couplings (between second-neighbor spins along one lattice direction). This competition leads to a series of commensurate and incommensurate modulated phases of arbitrarily long wavelength (see, e.g., [4]).

In this paper we show that a system where the spins tend to be aligned to the majority of their neighbors has a low temperature striped phase; this phenomenon is not pointed out by the ANNNI model and might lend some insight into the problem of the formation of stripelike patterns.

The model we propose here is an Ising model where the contribution of a given spin to the Hamiltonian is $-\beta$ if the spin is aligned to the majority of its neighbors and $+\beta$ if it is not. In the following we give the definition of the model that we are going to discuss. Let us consider the infinite bidimensional square lattice $\Lambda=\mathbf{Z}^2$ and define a $\mathbf{Z}_2$ spin variable $s_i\in\{-1,+1\}$ on each site $i\in\Lambda$. We denote by $s\in\Omega=\{-1,+1\}^{\Lambda}$ a configuration of the system and define the formal Hamiltonian

$$H(s)=-\beta\sum_{i\in\Lambda}s_i\phi_i(s), \tag{1}$$

where β is a positive real number and

$$\phi_i(s)=\mathrm{sgn}\left\{\sum_{j=1}^{9}s_{i,j}\right\}\quad\forall i\in\Lambda, \tag{2}$$

where we have denoted by $s_{i,j}$, $j=1,\ldots,9$, the nine spins in the 3×3 square block B_i centered on the site i. All the equilibrium properties of the model can be obtained from the partition function $Z_\Lambda(\beta)=\Sigma_{s\in\Omega}\exp[-H(s)]$.

If $\beta>0$ model (1) is characterized by a sort of ferromagnetic coupling among the spin variables. We remark that model (1) is ferromagnetic in a different fashion from the Ising model $H_I=-\beta\Sigma_{\langle i,j\rangle}s_is_j$ (where the sum runs over the pairs of nearest neighbor sites in Λ); we call this kind of coupling *ferromagnetic coupling with threshold*.

Indeed, let us suppose $s_i=+1$: in the Ising model the contribution of the spin s_i to the total energy of the system decreases when the number of nearest neighbor plus spins increases; hence by increasing the number of plus spins among s_i nearest neighbors we get more and more energetically preferable situations. In our model the contribution of the spin s_i to the total energy has only two possible values: $+\beta$ if the number of plus spins in B_i is less than 5 and $-\beta$ if it is greater than or equal to 5; hence, from the point of view of the spin s_i, the best situation is reached when four of the eight spins in $B_i\backslash\{i\}$ are equal to $+1$ and there is no further energetic gain if the number of plus spins in $B_i\backslash\{i\}$ increases up to 8.

As will be explained below, due to the freedom in the choice of number and location of the plus (minus) spins around a fixed plus (minus) one, our model shows a very peculiar behavior at low temperatures. In the following we give some evidence of a critical phase transition to a low temperature phase, which is a sort of ''polymer phase'' made of alternate stripes with fluctuating boundaries.

The occurrence of a striped phase does not depend on the geometry of the blocks B_i, which appear in the definition of model (1). We find a striped phase also for the model

$$\widetilde{H}(s)=-\beta\sum_{i\in\Lambda}s_i\widetilde{\phi}_i(s)\quad\forall s\in\Omega, \tag{3}$$

where β is the inverse temperature and

$$\widetilde{\phi}_i(s)=\mathrm{sgn}\left\{\sum_{j=1}^{5}s_{i,j}\right\}\quad\forall i\in\Lambda, \tag{4}$$

where we have denoted by $s_{i,j}$, $j=1,\ldots,5$, the five spins in the ''cross'' block C_i containing the site i and its four nearest neighbors.

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The Hamiltonian (1) is not strictly ferromagnetic; we mean that it does not satisfy the conditions under which Griffiths inequalities hold [5]. Indeed, by expanding H as a linear combination of products of the spin variables it can be shown that in model (1) the couplings between nearest and next to nearest neighbor spins are ferromagnetic, but antiferromagnetic terms are present as well; in the case of model (3) the coupling between nearest neighbors is ferromagnetic, while the coupling between next to nearest neighbors is antiferromagnetic. In both the models a competition between ferromagnetic and antiferromagnetic couplings occurs; this is similar to what happens in the case of the ANNNI model.

Due to this competition it is not surprising to find striped phases in our model. We remark that this competition is essentially an ''entropic'' effect. The spin s_i prefers to have just four parallel spins in $B_i\backslash\{i\}$: this is energetically equivalent to the situation with eight parallel spins in $B_i\backslash\{i\}$, but the former can be realized in many different ways, while the latter just in one way. The phase transition has been studied by a renormalization group transformation known as ''majority rule'' (see, e.g., [6,7]); this is suggested by the structure of Hamiltonian (1).

Model (1) has also an interesting interpretation as a ''model of atoms''; indeed, it can be seen as a model of a binary alloy, namely, a mixture of two species of atoms (say A and B), such as the Ising model (see, e.g., [8]). But in the present case the configurations which are energetically preferred are those in which an A (B) atom has at least four A (B) atoms among its nearest and next to nearest neighbors, no matter if the number of such atoms is greater than 4. Due to this fact the ordered phase is an alternate sequence of stripes of A and B atoms.

The transformation (2) is widely used for the recovering of noisy images and it is known as the *median filter* (see, e.g., [9]). It follows that the Hamiltonian (1) provides a stochastic version of the median filter.

Finally, we observe that in our model each spin is coupled to a Boolean function of its neighbor spins; this fact resembles the dynamical rules in the *random networks of automata*, where each spin is updated according to a random Boolean function of its neighbors (*finite dimensional case*) or to a random Boolean function of a certain number k of random spins of the whole network (*mean field case*; see [10]).

The paper is organized as follows: in the next section the expansion of Hamiltonians (1) and (3) in terms of products of spin variables is performed. In Sec. III the phase transition is studied by mapping the model onto the Ising version of the isotropic eight-vertex model. Section IV summarizes the conclusions.

II. SOME PROPERTIES OF THE HAMILTONIAN

In this section we discuss some properties of model (1); in particular, we describe its ground states, we give a rough evaluation of its residual entropy, and we expand its Hamiltonian as sums of products of the spin variables.

Model (1) has an infinite number of ground states, which are the configurations satisfying the constraint

$$s_i = \phi_i(s) \quad \forall i \in \Lambda; \tag{5}$$

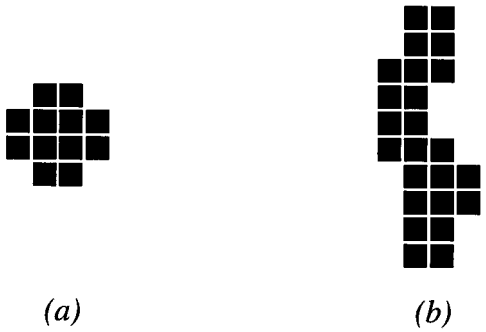


FIG. 1. (a) The smallest cluster invariant to the transformation (2): black squares represent plus spins on a minus background or, vice versa, minus spins on a plus background. (b) A portion of a polymer. The polymer is supposed to be infinitely long; it satisfies the constraint (5), as well.

such configurations are called *median roots*, that is, configurations invariant under the median filtering.

A complete characterization of bidimensional median roots is still missing. We refer to [9] for a related discussion and describe them heuristically: a median root is made of two typical kinds of structures, namely, clusterlike structures and polymerlike structures. In Fig. 1(a) we show the smallest cluster which is a root, a 12-spin cluster called *minroot*, while in Fig. 1(b) a typical polymer structure is depicted.

It follows that the model has a residual entropy; we obtain a rough estimate of it by considering the model defined on a cylinder of $6\times N$ sites with $N\to\infty$. On a $6\times N$ strip (with periodic boundary conditions in the six-site direction) we can classify the median roots by the configurations in the last two columns. Taking into account the symmetries of the problem (parity $s\to -s$ and invariance under rotations of the cylinder) leads to 30 nonequivalent classes. A 30×30 transfer matrix $T_{a,b}$ can be defined as the number of a roots on the $6\times(N+1)$ cylinder obtained by any b root on the $6\times N$ cylinder by adding a column.

The largest eigenvalue of the transfer matrix provides the residual entropy. We do not report the details here, but only quote the results. The largest eigenvalue is found to be $\lambda_0 = 3.574\,77$ and the residual entropy per site $1/6\,\ln\lambda_0 = 0.212\,32$. To our knowledge there is not any estimate in the literature for the entropy of the median roots to compare with ours.

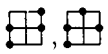
In order to expand Hamiltonian (1) as a linear combination of products of the spin variables we recall that if $f(s)$ is a function of the $\mathbf{Z}_2$ spin variables s_i where i ranges over some finite set V, then $f(s)$ may be written in a unique way as

$$f(s) = \sum_X c(X) s(X), \tag{6}$$

where $s(X) = \Pi_{i\in X} s_i$, the sum runs over all the subsets $X \subset V$, and the numbers $c(X)$ are given by

$$c(X) = \frac{1}{2^{|V|}} \sum_{s\in\{-1,+1\}^V} s(X) f(s), \tag{7}$$

TABLE I. The coefficients γ_i, introduced in Eq. (8), are listed. In the third column the families Γ_i, to which each coefficient γ_i is related, are briefly described. In the fourth column a typical set $\zeta \in \Gamma_i$ is depicted: the grid represents the 3×3 block B in which ζ is contained; the sites of B belonging to ζ are represented by the black circles. We remark that just an example of set belonging to Γ_i is depicted in the fourth column; for example, in the case $i=10$ one can consider the following sets, as well:



i	γ_i	description of Γ_i	typical cluster in Γ_i
1	+200	pairs of nearest neighbors sites	
2	+240	pairs of next to the nearest neighbors sites	
3	-60	pairs of second–neighbor sites along the lattice directions	
4	-40	two–site clusters with sites at distance $\sqrt{5}$ lattice spacings	
5	-20	pairs of second–neighbor sites along the lattice diagonals	
6	-80	plaquettes	
7	-40	four–site clusters containing the center of the block B and occupying a 3×2 rectangular block	
8	-20	four–site clusters containing the center of the block B and occupying the whole B	
9	+24	four–site clusters not containing the center of the block B and occupying a 3×2 rectangular block	
10	+12	four–site clusters not containing the center of the block B and occupying the whole B	
11	+12	six–site clusters containing the center of the block B and occupying the whole B	
12	+24	six–site clusters containing the center of the block B and occupying a 3×2 rectangular block	
13	-20	six–site clusters not containing the center of the block B and, necessarily, occupying the whole block B	
14	-20	eight–site clusters containing the center of the block B	
15	+140	eight–site clusters not containing the center of the block B	

where $|V|$ is the cardinality of V, that is, the number of sites in V.

Now, we observe that H can be written as follows:

$$H(s)=-\beta\sum_{i\in\Lambda} f_i(s), \tag{8}$$

where the function $f_i(s)=s_i\phi_i(s)$ is defined on the finite sets $B_i\ \forall i\in\Lambda$. Hence, the function $f_i(s)$ can be expanded as in Eq. (6): one has to calculate $2^9-1=511$ coefficients (that is, one has to consider all the possible subsets of B_i except for the empty set). This number could be reduced by taking properly into account the symmetries of the Hamiltonian.

We have performed a computer assisted calculation of all the coefficients and, by working out the sums in Eq. (8), we have obtained

$$H(s)=-\frac{\beta}{2^9}\sum_{i=1}^{15}\gamma_i\sum_{\zeta\in\Gamma_i} s(\zeta), \tag{9}$$

where the families Γ_i of subsets of B_i and the related coefficients γ_i are given in Table I. We remark that each Γ_i represents a family of a certain kind of sets of sites of Λ contained in a 3×3 block B; for example, Γ_1 is the family of all the pairs of nearest neighbor sites and Γ_6 is the family of all the plaquettes.

This calculation shows that model (1) is not ferromagnetic (see Table I) in the sense that it does not fulfill the hypothesis under which Griffiths inequalities hold. This model is characterized by ferromagnetic and antiferromagnetic couplings: we observe that the two-spin interactions are ferromagnetic if two adjacent columns or rows are involved (nearest and next to nearest spin couplings), while they are antiferromagnetic if the involved columns or rows are at a distance of two lattice spacings. As in the case of the ANNNI model, one may expect that the result of this competition could be a low temperature striped phase.

By performing the same calculation in the case of model (3) we have obtained

$$\widetilde{H}(s)=-\frac{\beta}{2^5}\Bigg[24\sum_{\langle i,j\rangle}s_is_j-8\sum_{\langle\langle i,j\rangle\rangle}s_is_j-4\sum_{\langle\langle\langle i,j\rangle\rangle\rangle}s_is_j$$
$$-4\sum_{\mathrm{T}_{i,j,k,l}}s_is_js_ks_l+12\sum_{\diamond_{i,j,k,l}}s_is_js_ks_l\Bigg], \tag{10}$$

where the five sums run, respectively, over the pairs of nearest neighbors, the pairs of next to nearest neighbors, the pairs of second neighbors along the lattice directions, the four-site cluster containing a site i and three of its four nearest neighbors (**T**-shaped clusters), and the square four-site clusters with sides at 45° with respect to the lattice directions. Even model (3) exhibits a competition between ferromagnetic and antiferromagnetic couplings; hence we expect a low temperature striped phase in this case, as well.

III. THE PHASE TRANSITION

The structure of Hamiltonian (1) suggests the introduction of a new set of dynamical variables in order to investigate the phase diagram of our model.

Suppose we partition Λ into 3×3 squared blocks B_α where α is the site that is in the center of B_α; the collection of all these sites α is denoted by Λ'. On each of these sites α we define the new variable

$$s'_\alpha=\phi_\alpha \quad \forall\alpha\in\Lambda'; \tag{11}$$

we have defined the new variables by ''integrating'' over the fluctuations of the old ones on square 3×3 blocks: we expect that the details of the configurations of the system on the scale of three lattice spacings are inessential to describe the peculiarities of the ordered phase.

We have, then, introduced a new model defined on the lattice Λ', with space of configurations $\Omega'=\{-1,+1\}^{\Lambda'}$; the equilibrium (unnormalized) measure of this new model is given by

$$\mu'(s')=\sum_{s\in\Omega}Z(s',s)e^{-H(s)}, \tag{12}$$

where the probability kernel $Z(s',s)=\Pi_{\alpha\in\Lambda'}\delta_{s'_\alpha,\phi_\alpha(s)}$ has been introduced. The formal Hamiltonian of the new model is

$$H'(s')=-\ln\mu'(s')+\text{const} \quad \forall s'\in\Omega'. \tag{13}$$

In order to work out the sum in Eq. (12) we use the method of the cumulant expansion (see [11]), writing Hamiltonian (1) in the form $H(s)=H_0(s)+V(s)\forall s\in\Omega$, where $H_0(s)=-\beta\Sigma_{\alpha\in\Lambda'}s_\alpha\phi_\alpha(s)$ contains the interactions be-

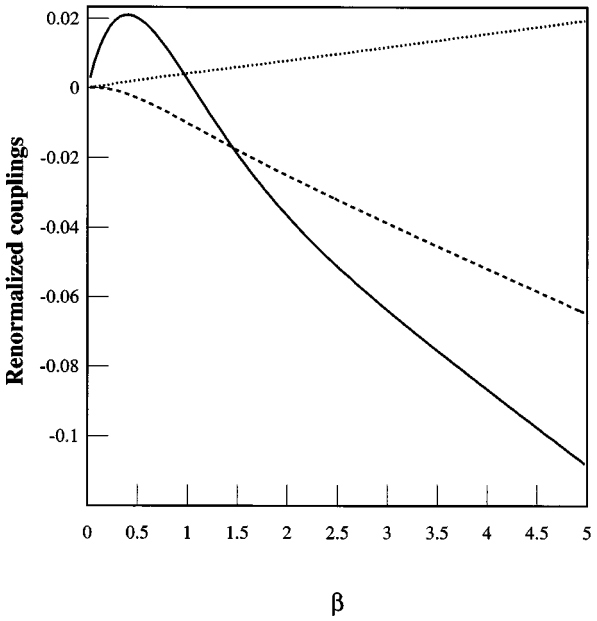


FIG. 2. Renormalized couplings as functions of β in the case of model (1). Solid, dashed, and dotted lines represent, respectively, $J_{\langle\ \rangle}$, $J_{\langle\langle\ \rangle\rangle}$, and $J_{\square}$.

tween spins within the same block $B_\alpha \forall \alpha \in \Lambda'$, while $V(s) = -\beta \Sigma_{i \in \Lambda \setminus \Lambda'} s_i \phi_i(s)$ contains the interactions between spins belonging to different blocks. By truncating the cumulant expansion at the first order, one can show that the new Hamiltonian is in the form

$$-H'(s') = \text{const} + J_{\langle\ \rangle} \sum_{\langle \alpha\gamma \rangle} s'_\alpha s'_\gamma + J_{\langle\langle\ \rangle\rangle} \sum_{\langle\langle \alpha\gamma \rangle\rangle} s'_\alpha s'_\gamma + J_\square \sum_{\substack{\gamma \\ \alpha \square \delta \\ \eta}} s'_\alpha s'_\gamma s'_\delta s'_\eta, \tag{14}$$

where the three sums run, respectively, over all the pairs of nearest neighbors and next to nearest neighbors and over all the plaquettes in Λ'; we remark that the new model is the Ising version of the isotropic eight-vertex model [1]. With a computer assisted calculation we have obtained the new couplings $J_{\langle\ \rangle}, J_{\langle\langle\ \rangle\rangle}$, and $J_\square$ as functions of the original coupling β (see Fig. 2); their structure is $J_a(\beta) = \beta F_a(e^{2\beta})$, where F_a are rational functions.

The variables transformation (11) and the calculation of the Hamiltonian of the new model amount to performing the ''majority rule'' renormalization group transformation (see [6,7]). We remark that for β large enough, with a single step of renormalization, model (1) is mapped into the eight-vertex model (14) with ''negative'' nearest and next to nearest neighbor couplings; that is, starting from a model which is in some sense ferromagnetic, we obtain a model with antiferromagnetic couplings.

The phase diagram of the eight-vertex model is well known (see, e.g., [1,7,12]): at $J_{\langle\langle\ \rangle\rangle} < 0$ and $|J_{\langle\ \rangle}| < 2|J_{\langle\langle\ \rangle\rangle}|$ this phase diagram is characterized by a critical surface separating the paramagnetic and the superantiferromagnetic (SAF) phases; respectively, the high and the low temperature

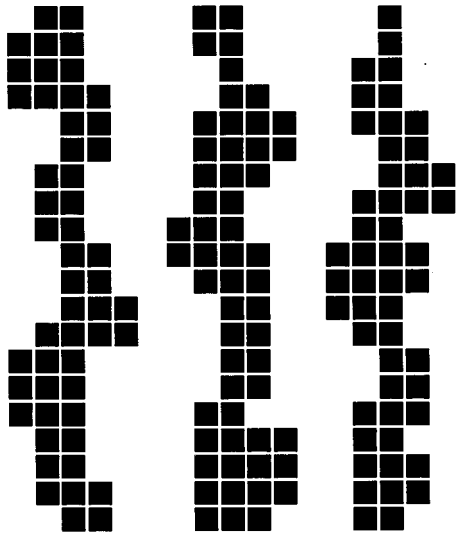


FIG. 3. The typical low temperature pattern for our model. The average distance between polymers of the same sign is six lattice spacings. The constraint (5) is almost satisfied.

phases. We observe that as β increases from zero to infinity the renormalized eight-vertex model (14) undergoes a second-order phase transition from the paramagnetic to the SAF phase.

Hence, there exists a value β_c such that at $\beta = \beta_c$ our original model is ''critical''; the high temperature phase is the usual paramagnetic phase: what about the low temperature one? In terms of the new variables s'_α with $\alpha \in \Lambda'$ this phase can be characterized by a staggered magnetization m' defined as the difference between the magnetization on even and odd columns: $m' = 0$ in the paramagnetic phase, $m' \neq 0$ in the SAF phase. But a column of the new model corresponds to a strip of length three lattice spacings in model (1); then, at low temperature, model (1) exhibits an ordered phase made of an alternate sequence of parallel plus and minus polymers, infinitely long and three lattice spacings wide (see Fig. 3). This suggests that the median roots are entropically dominated by polymer–like structures developing parallel to one of the lattice directions.

We have studied model (3) following the scheme used for model (1); we have partitioned the lattice Λ as in Fig. 4. The Hamiltonian associated with the block variables is

$$-\widetilde{H}'(s') = \text{const} + \widetilde{J}_{\langle\ \rangle} \sum_{\langle \alpha\gamma \rangle} s'_\alpha s'_\gamma + \widetilde{J}_{\langle\langle\ \rangle\rangle} \sum_{\langle\langle \alpha\gamma \rangle\rangle} s'_\alpha s'_\gamma \tag{15}$$

with $\widetilde{J}_{\langle\ \rangle}$ and $\widetilde{J}_{\langle\langle\ \rangle\rangle}$ depending on β as in Fig. 5.

Even for model (3) the renormalized model exhibits a low temperature SAF phase. Due to the geometry of the cross blocks, in this case the polymers of the low temperature phase are parallel to the dashed lines depicted in Fig. 4.

IV. CONCLUSIONS

We have proposed an Ising-like spin model with a new kind of coupling in order to point out that a simple request, such as the tendency of each spin to be aligned to the ma-

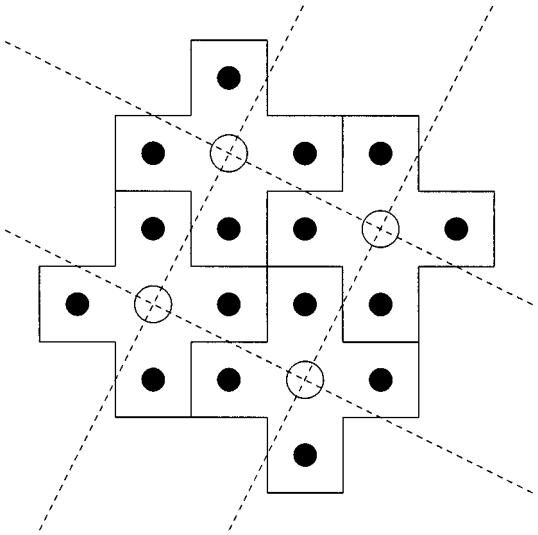


FIG. 4. The partition of the lattice used to study model (3). The renormalized variables are defined on the blank circles, which form the new lattice.

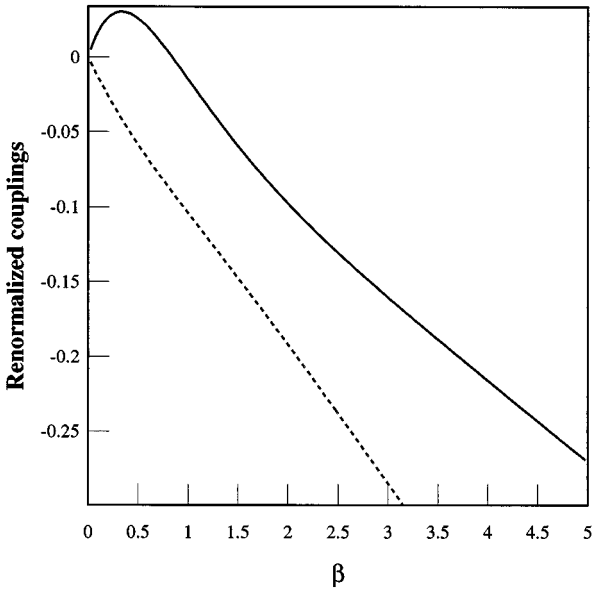


FIG. 5. Renormalized couplings as functions of β in the case of model (3). Solid and dashed lines represent, respectively, $\widetilde{J}_{\langle\ \rangle}$ and $\widetilde{J}_{\langle\langle\ \rangle\rangle}$.

jority of its neighbors, leads to low temperature striped phases.

The expansion of the Hamiltonian in terms of products of spin variables pointed out the similarities between our model and the ANNNI model; this suggests the hypothesis that the model undergoes a phase transition to a striped phase.

We studied the model by renormalization group methods and at the level of approximation we have considered, first order of cumulant expansion, the phase transition is observed.

The parallel polymerization appears to be characteristic of a ferromagnetic coupling with threshold. In the spirit of the ''atomic'' interpretation, this implies that the clusters of A atoms, as well as B atoms, become one-dimensional at low temperature, i.e., they lose one dimension.

Our estimations of critical couplings are $\beta_c \sim 25$ for model (1) and $\beta_c \sim 5$ for model (3). The cumulant expansion is known to be relevant near the critical point. A low temperature series expansion would better describe the model in the limit $\beta \to \infty$; this is not a trivial task, since a rigorous analysis of the statistical properties of the ground states is needed. This will be the topic of further work.

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