

# Nature of phase transitions in the striped phase of a triangular-lattice Ising antiferromagnet

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Different scenarios of the fluctuation-induced disordering of the striped phase which is formed at low temperatures in the triangular-lattice Ising model with the antiferromagnetic interaction of nearest and further neighbors are analyzed and compared. The dominant mechanism of the disordering is related to the formation of a network of domain walls, which is characterized by an extensive number of zero modes and has to appear via the first-order phase transition. In principle, this first-order transition can be preceded by a continuous one, related to the spontaneous formation of double domain walls and a partial restoration of the broken symmetry, but the realization of such a scenario requires the fulfillment of rather special relations between the coupling constants.

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## I. INTRODUCTION

An Ising model can be defined by the Hamiltonian

$$H = \sum_{(i,j)} J_{ij} \sigma_i \sigma_j, \quad (1)$$

where the fluctuating variables (spins),  $\sigma_j = \pm 1$ , are defined on the sites  $\mathbf{j}$  of some regular lattice. In the standard version of the model<sup>1-3</sup> the coupling constants,  $J_{ij}$ , are assumed to be nonzero only when  $\mathbf{i}$  and  $\mathbf{j}$  are the nearest neighbors of each other, but in a more general case one can suppose that they depend on the distance between  $\mathbf{i}$  and  $\mathbf{j}$ . The models belonging to this class play an extremely important role in the condensed matter physics, because they can be used for the description of a huge variety of systems with a twofold degeneracy of an order parameter. The best known examples of such systems are ferromagnets and antiferromagnets with strong easy axis anisotropy and adsorbed monolayers.

The exact solution of the Ising model on a triangular lattice with the interaction of only nearest neighbors was found in 1950.<sup>2,3</sup> In the case of the isotropic antiferromagnetic interaction it demonstrates rather unusual properties. Namely, the system remains disordered at arbitrarily low temperature<sup>2,3</sup> and at zero temperature is characterized by an algebraic decay of the correlation functions<sup>4,5</sup> and a finite residual entropy per site.<sup>2</sup> The ground states of this model can be mapped<sup>6</sup> onto the states of a solid-on-solid (SOS) model describing the fluctuations of the (111) facet of a crystal with a simple cubic lattice (as well as on the states of the dimer problem on a honeycomb lattice<sup>7</sup>) and are infinitely degenerate.

This degeneracy is not related to symmetry and therefore in a physical situation its removal by the interactions of more distant neighbors should be taken into account. If the interaction of second neighbors (characterized by the coupling constant  $J_2$ ) is included into consideration, for both signs of  $J_2$  the degeneracy of the ground states is reduced to a sixfold one.<sup>8</sup> In terms of the SOS representation,<sup>6</sup> the ferromagnetic interaction of second neighbors ( $J_2 < 0$ ) corresponds to the positive energy of a step and, therefore, leads to the stabilization of the flat phase at low enough temperatures.<sup>9</sup> With

the increase of temperature a roughening transition<sup>10</sup> takes place, which at a higher temperature is followed by another phase transition related to the dissociation of pairs of dislocations.<sup>9,11</sup> Both transitions belong to the Berezinskii-Kosterlitz-Thouless universality class.

This scenario follows also from approximate mappings<sup>12,13</sup> of the considered model onto a six-state clock model and has been confirmed by numerous Monte Carlo simulations.<sup>11,13,14</sup> As is typical for low-dimensional systems, a mean field analysis<sup>15</sup> leads to the wrong conclusions about the character of the intermediate phase or the nature of phase transitions.

The present work is devoted to the antiferromagnetic Ising model on a triangular lattice in which the interaction of second neighbors is also antiferromagnetic. For brevity we shall call such a system a triangular-lattice Ising antiferromagnet. The structure of the ground state of the triangular-lattice Ising antiferromagnet with the interaction of first and second neighbors<sup>8</sup> is shown in Fig. 1. Here and below filled and empty circles are used to denote the spins of different signs.

Although this version of the Ising model have been also investigated by different methods,<sup>16-19</sup> its properties are not as clearly understood as those of the model with the ferromagnetic interaction of second neighbors. In particular, Domany *et al.*<sup>16</sup> have demonstrated that the construction of the Ginzburg-Landau functional describing the formation of the state whose structure is shown in Fig. 1 reproduces the Hamiltonian of the Heisenberg model with the cubic anisotropy, which under the renormalization is transformed<sup>20</sup> into the discrete cubic model.<sup>21</sup> However, this hardly allows one

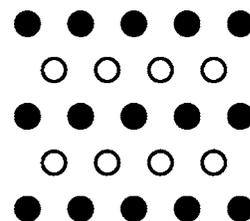


FIG. 1. The structure of the ground state for  $J_{1,2} > 0$ .

to make any conclusions about the properties of a triangular-lattice Ising antiferromagnet (i) because the cubic model allows for *three* different scenarios of disordering<sup>22</sup> (although sometimes only one of them is mentioned<sup>23</sup>), and (ii) because this approach does not take into account the strong chiral asymmetry<sup>24</sup> existing in the problem (see Sec. II for more details). Additionally, such a description cannot reproduce the well-known properties of the model with only first-neighbor interaction. The same can be also said about the mean-field approach of Kaburagi *et al.*,<sup>17</sup> which gives an unrealistic prediction of a three-sublattice intermediate phase.

A more direct analysis of the fluctuations which can be responsible for the disordering of the striped phase has been undertaken by Hemmer *et al.*<sup>18,19</sup> However, these authors have considered the formation of only one type of domain walls, whose appearance (as is discussed in Sec. III) can lead only to a *partial* restoration of the broken symmetry. Thus, all conclusions of Refs. 18 and 19 are based on the essentially incomplete physical picture and have to be reconsidered.

This article is devoted to comparison of different mechanisms and different scenarios of disordering which are possible in the striped phase of a triangular-lattice Ising antiferromagnet. Although a number of numerical works<sup>25–27</sup> give evidence on the existence of a single first-order transition (for this or that choice of the relation between the coupling constants), in a situation when different mechanisms of disordering compete with each other one hardly can be sure about the universality of this result.

Our analysis assumes that  $J_1$  is much larger than all other coupling constants, which allows one to use the approaches relying on the separation of different energy scales. This limit is also of interest because it corresponds to the case of strong chiral asymmetry and is the most relevant one for many physical realizations of the model. The outlook of the article is as follows.

In Sec. II we discuss the symmetry of the ground states and the structure of domain walls and estimate the temperature at which the free energy of a single domain wall vanishes as a result of thermal fluctuations of this wall. In Sec. III we show that the free energy of a double domain wall can be expected to vanish at much lower temperature than that of a single wall, and argue that this suggests a possibility of a two-transition scenario.

In Sec. IV the spontaneous formation of a network of single domain walls is analyzed. In the limit when this network has to be diluted, it becomes clear that it has to appear via a first-order phase transition. When only the interaction of up to third neighbors is taken into account, the estimates for the temperatures of this transition and of the spontaneous formation of double domain walls coincide with each other, which suggests that there is only one phase transition in the system. In Sec. V a phenomenological free-energy functional is constructed which allows one to confirm that the transition to the disordered phase has always to be of the first order.

The interplay between the two main mechanisms of the disordering is analyzed in Sec. VI, whereas the results are summarized in Sec. VII. The short Appendix is devoted to a formal derivation of an exact upper boundary for the tem-

perature at which the long-range order in  $\sigma_j$  is destroyed by thermal fluctuations when  $J_1 = \infty$ .

## II. GROUND STATES AND DOMAIN WALLS

The structure of the ground state of the triangular-lattice Ising model with the antiferromagnetic interaction of nearest and second neighbors<sup>8</sup> is shown in Fig. 1, whereas Fig. 2 illustrates the classification of neighbors on a triangular lattice according to their distance from a given cite (denoted by zero). In the following we assume that  $J_3$ , the coupling constant describing the interaction of third neighbors, can also be nonzero, but satisfies the constraint,<sup>28,29</sup>  $J_3 < J_2/2$ , which is required for the stability of the striped ground state of Fig. 1. The role of the interactions of more distant neighbors will be discussed in Sec. VI. To make a situation more transparent we assume that the interaction of nearest neighbors,  $J_1$ , is much larger than all other coupling constants.

The sixfold degeneracy of the state shown in Fig. 1 corresponds to the violation of the  $Z_2 \times Z_3$  symmetry, where  $Z_2$  is related to the possibility of interchanging positive and negative spins, and  $Z_3$  to three possible orientations of the stripes formed by spins of the same sign. Each of the six ground states can be associated with a unit vector pointing either in positive or negative direction along one of the three axes, which are perpendicular to each other. These six directions can also be put into correspondence with the six faces of a cube. In such a representation the group  $Z_2$  is related to the reflection symmetry which transforms the opposite faces of a cube into each other, whereas the group  $Z_3$  corresponds to the cyclic permutations of the three axes.

In systems with a discrete degeneracy the destruction of a long-range order has to be driven by thermal activation of infinite domain walls. The appearance of a sequence of more or less parallel walls is expected when the intersections of walls with different orientations are energetically unfavored.<sup>30</sup> The alternative option consists of the appearance of a network of intersecting domain walls with different orientations, which would be favored by a negative energy of domain wall intersections.<sup>30</sup>

Figure 3(a) shows an example of a lowest-energy domain wall separating two different ground states. Each segment of such a wall connects two neighboring spins of the opposite signs and separates two second neighbors of the same sign. The energy of this wall per unit length,

$$E_{dw} = 2J_2 - 4J_3 > 0,$$

does not depend on  $J_1$ , because its presence does not lead to the violation of the constraint

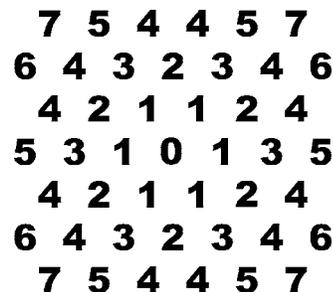


FIG. 2. The classification of neighbors on triangular lattice.

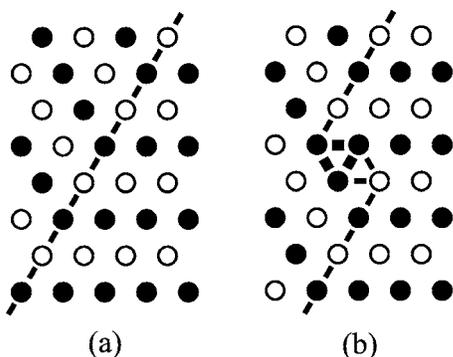


FIG. 3. Low energy domain walls: (a) a straight one; (b) with a kink.

$$\sigma_j \sigma_{j'} + \sigma_{j'} \sigma_{j''} + \sigma_{j''} \sigma_j = -1 \quad (2)$$

on any triangular plaquette. This condition is satisfied when a plaquette contains spins of both signs.

When crossing a domain wall the direction of the stripes formed by the spins of the same sign changes by  $60^\circ$  and, therefore, the direction of a lowest-energy wall is uniquely determined by the pair of ground states which it separates. In other terms, the energy of a domain wall in the considered model is strongly dependent both on its orientation and on which states it separates. From the analysis of systems with a threefold degeneracy it is known that such a property (the chiral asymmetry<sup>24</sup>) can lead to the change of the universality class<sup>33</sup> or even of the order<sup>34-36</sup> of a phase transition. This is the reason why the analogy with the cubic model<sup>21,22</sup> without chiral asymmetry (which follows from the Landau-Ginzburg analysis of Domany *et al.*<sup>16</sup>) is insufficient for understanding the properties of a triangular-lattice Ising antiferromagnet with  $J_{2,3} \ll J_1$ .

Any fluctuations of domain wall are impossible without the violation of the constraint (2), and therefore require the energies proportional to  $J_1 \gg E_{dw}$ . Figure 3(b) shows an example of the simplest elementary defect (a kink) which can be formed on a straight domain wall. The energy of such a defect,

$$E_k = 2J_1 - 4J_3,$$

has to include a contribution proportional to  $J_1$ , because the formation of a kink requires to have one plaquette at which all three spins are of the same sign, and therefore

$$\sigma_j \sigma_{j'} + \sigma_{j'} \sigma_{j''} + \sigma_{j''} \sigma_j = 3.$$

In Fig. 3(b) this plaquette is shown by bold lines.

At finite temperatures the free energy of a domain wall (per unit length) can be estimated as the difference between its energy and the entropic term related to the formation of kinks.<sup>31</sup> For  $T \ll E_k$  this gives

$$F_{dw}(T) \approx E_{dw} - 2T \exp(-E_k/T). \quad (3)$$

It is well known that when the intersections of domain walls are unfavored, one can expect the formation of a dilute sequence of parallel (on the average) walls when the free

energy of a single wall,  $F_{dw}(T)$ , becomes equal to zero.<sup>30,32</sup> For  $F_{dw}(T)$  defined by Eq. (3) this takes place at

$$T = T_1 \approx \frac{E_k}{\ln(E_k/E_{dw})} \quad (4)$$

where we have taken into account that  $E_{dw} \ll E_k$  (as a consequence of  $J_2 \ll J_1$ ). Equation (4) shows that for  $J_2, J_3 \ll J_1$  the temperature  $T_1$  only weakly depends on  $J_2$  and  $J_3$  and is determined mainly by  $J_1$ .

In the limit  $J_1 \rightarrow \infty$  the fluctuation-induced vanishing of the free energy of a single domain wall becomes impossible. This manifests itself in the divergence of the expression for  $T_1$  given by Eq. (4) for  $E_k \rightarrow \infty$ . Quite remarkably, even in this limit there still remain possibilities for a fluctuation-induced destruction of the long-range order. They are related to the spontaneous formation of *double* domain walls (which is discussed in Sec. III) and of a domain-wall network (discussed in Sec. IV).

### III. SPONTANEOUS FORMATION OF DOUBLE DOMAIN WALLS

A double domain wall consists of two parallel single walls [see Fig. 4(a)] and separates two ground states with the same direction of spin stripes. The energy of a straight double wall per segment,  $E_{ddw}$ , is given simply by the energy of two single domain walls from which it consists,  $E_{ddw} = 2E_{dw}$ . The interaction between two parallel single walls does not appear even if one takes into account the interactions of spins with their fourth and fifth neighbors (see Fig. 2). However, it turns out that the fluctuations of a double wall cost less energy than those of a single wall, as a consequence of which its free energy can easily become smaller than that of a single wall.

Figure 4(b) demonstrates that the fluctuations of a double domain wall are possible without the violation of the constraint (2). From this figure it is clear that each corner on a double wall requires the appearance of an additional segment of a single domain wall. The energy of such a defect,  $E_c = 2J_2$ , does not depend on  $J_1$  and  $J_3$ . At finite temperatures the expression for the free energy of a double wall which takes into account the presence of thermally activated corners is of the form<sup>19,37</sup>

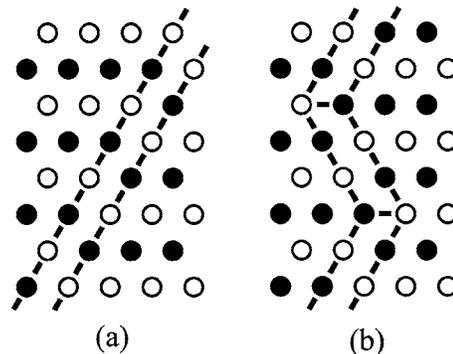


FIG. 4. Double domain walls: (a) straight; (b) with two corners.

$$F_{\text{ddw}}(T) = 2E_{\text{dw}} - T \ln[1 + \exp(-E_c/T)]. \quad (5)$$

The spontaneous appearance of a diluted sequence of such walls can be expected to take place when  $F_{\text{ddw}}(T)$  becomes equal to zero. The condition  $F_{\text{ddw}}(T)=0$  can be rewritten as

$$T = \frac{E_c}{-\ln[\exp(2E_{\text{dw}}/T) - 1]}. \quad (6)$$

Note that Eq. (6) and, therefore, its solution,  $T_2$ , do not depend on  $J_1$ .

In the case of  $J_3=0$  the solution of Eq. (6) gives

$$T_2 = \gamma_2 J_2 \quad (7)$$

where<sup>19,37</sup>

$$\gamma_2 = \frac{1}{2} \ln \left[ \left( \frac{1}{2} + \sqrt{\frac{23}{108}} \right)^{1/3} + \left( \frac{1}{2} - \sqrt{\frac{23}{108}} \right)^{1/3} \right] \approx 7.112$$

whereas for  $E_{\text{dw}} \ll E_c$  an expansion of the exponent in the right-hand side of Eq. (6) allows one to find that

$$T_2 \approx \frac{E_c}{\ln(E_c/2E_{\text{dw}})} \approx \frac{2J_2}{\ln(J_2/2E_{\text{dw}})}. \quad (8)$$

Comparison of Eqs. (7) and (8) with Eq. (4) demonstrates that for  $J_2 \ll J_1$  the destruction of the long-range order in  $\sigma_j$  cannot be driven by the spontaneous formation of a sequence of single domain walls, because the analogous sequence of double domain walls can be expected to appear at much lower temperature. A numerical calculation of  $T_2$  for an arbitrary relation between  $J_1$  and  $J_2$  (at  $J_3=0$ ) in terms of the one-dimensional SOS model which takes into account also more complex fluctuations of a double domain wall can be found in Ref. 18.

In the limit  $J_1 \rightarrow \infty$  at low temperatures the system has to be completely frozen in one of its ground states, because any finite size fluctuation on the background of the striped ground state requires the violation of the constraint (2) on at least two plaquettes (see Fig. 5). Accordingly, the exact expression for the free energy of a double domain wall cannot contain any additional contributions related to the suppression of finite size fluctuations. This has allowed Shi and Wortis<sup>37</sup> to conjecture that in the limit  $J_1 \rightarrow \infty$  the condition  $F_{\text{ddw}}(T)=0$  [with  $F_{\text{ddw}}$  given by Eq. (5)] determines the *exact*

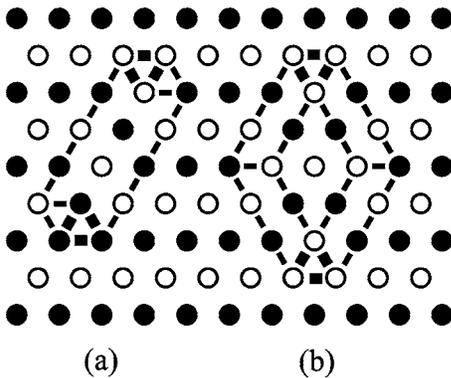


FIG. 5. Closed loops formed by (a) single domain walls, (b) double domain walls.

value of the transition temperature. However, this conclusion can be valid only if the spontaneous formation of a diluted sequence of double domain walls is not preceded by the spontaneous formation of a network of single domain walls (see Sec. IV).

It is rather evident that the average direction of a fluctuating double wall containing thermally activated corners will be perpendicular to the direction of spin stripes on both its sides. The spontaneous formation of a sequence of such walls leads to the restoration of the  $Z_2$  symmetry between the two states with the same direction of stripes and the reduction of the broken symmetry to  $Z_3$ .

Since the concentration of walls,  $\nu(T)$ , is restricted by their collisions (which are responsible for the reduction of the entropy of their fluctuations), Shi and Wortis<sup>37</sup> have concluded that this phase transition is continuous and belongs to the Pokrovsky-Talapov<sup>32</sup> universality class. Accordingly, in the vicinity of  $T_2$  one should have  $\nu(T) \propto (T-T_2)^{1/2}$ . Note that the value of the correlation length describing the decay of the correlation function  $\langle \sigma_i \sigma_j \rangle$  in the direction along the stripes is inversely proportional to  $\nu(T)$ .

On the other hand, Einevoll and Hemmer<sup>19</sup> have argued that this phase transition cannot be continuous, because the temperature at which  $F_{\text{ddw}}(T)$  vanishes is different for different directions of a double wall. In our opinion the latter conclusion is completely unjustified. The dependence of  $F_{\text{ddw}}$  on the direction of the wall manifests itself in the spontaneous formation of a sequence of walls with the same (on the average) direction, and is a *necessary condition* for the applicability of the Pokrovsky-Talapov theory<sup>32</sup> rather than an obstacle for its validity.

If one assumes that the value of  $J_1$  is finite, but large in comparison with  $J_2$ , the fluctuations in the low temperature phase become possible. Each point where a pair of single walls is created (or annihilates) cost the energy close to  $2J_1$ , so at low temperatures there will exist a finite concentration of highly anisotropic loops formed by such walls [see Fig. 5(a)]. However, at  $T \approx T_2 \ll J_1$  the average distance between them will be much smaller than their size, as a consequence of which their presence can be neglected. On the other hand, the size of the closed loops formed by double domain walls [see Fig. 5(b)] diverges when  $T \rightarrow T_2$ . From the theory of the commensurate-incommensurate transition it is known<sup>38</sup> that this is accompanied by the change of the type of the phase transition from the Pokrovsky-Talapov universality class<sup>32</sup> to that of the Ising model. However, the behavior will be changed only in a narrow region around  $T_2$ , which will be exponentially small in  $J_1/T_2$ .

Since the considered phase transition is related to the restoration of  $Z_2$  symmetry, the emergence of the Ising critical behavior looks rather natural. The different universality class in the case of  $J_1 = \infty$  can be explained by the extremely anisotropic nature of domain walls in that limit, which prevents the merging of different domains of the same state.

If the spontaneous formation of a sequence of double domain walls indeed takes place as a separate phase transition it has to be followed (with a further increase of temperature) by a second phase transition related to the restoration of  $Z_3$  symmetry. The completely disordered phase above this transition

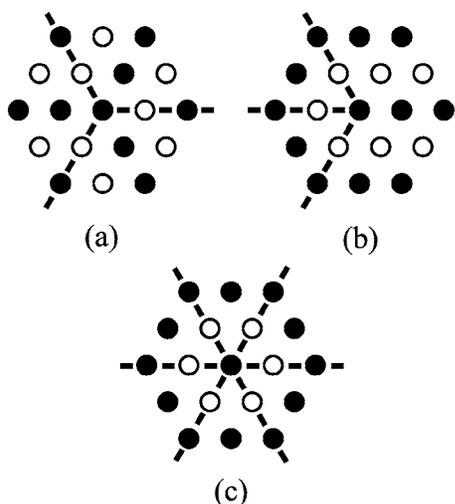


FIG. 6. Three low-energy domain walls with different orientations can merge or intersect with each other.

will look like a mixture of finite domains of all six ground states. Since double walls do not change the orientation of stripes, the second phase transition requires the formation of single domain walls of all possible orientations. Above we have found that the spontaneous formation of double domain walls takes place when the free energy of a single wall is still much larger than temperature, so it looks rather plausible that the two phase transition may be well separated from each other. However, to check if it is really so, the formation of a network of single domain walls has to be studied in more detail.

#### IV. SPONTANEOUS FORMATION OF A DOMAIN-WALL NETWORK

Like in the previous section it will be convenient to start by considering the case of  $J_1 = \infty$ . In this limit all single domain walls have to be straight due to the absence of kinks.

Figure 6 shows how such walls can intersect or merge with each other without violating the constraint (2). The energy of these intersections does not depend on  $J_1$  or  $J_2$ . In particular, the energy of the  $120^\circ$  junction shown in Fig. 6(a) is simply equal to zero,  $E_a = 0$ , whereas for the  $60^\circ$  junction shown in Fig. 6(b) it is given by  $E_b = 4J_3$ . The intersection shown in Fig. 6(c) can be considered as an overlap of two  $60^\circ$  junctions. The energy of this object is equal to  $E_* = 12J_3$ .

An important feature (already mentioned in Sec. II), which plays a crucial role in determining the structure of a domain-wall network for  $J_1 = \infty$ , is that the direction of each wall is uniquely determined by the states which it separates. A possible structure of a network which is formed by straight walls and satisfies this criterion is schematically shown in Fig. 7. Here the letters A, B, and C are used to denote the domains with three different orientations of stripes. Note that all walls between A and B are parallel to each other. The same is true for all walls between B and C, as well as for all walls between C and A.

For the sake of clearness we have not shown in Fig. 7 which of the two versions of A, of B, or of C (related to the change of sign of all spins) is realized in each particular domain. This depends on the exact positions of domain walls.

The structure of the network shown in Fig. 7 has been chosen to maximize the entropy for the given total length of the walls. The network of such a kind is characterized by a large number of zero modes which do not change its energy. For example, each domain of the type A can be moved to the left or to the right. This changes the areas of all domains of the types B and C which are adjacent to it, but the total length of domain walls (and, therefore, the total energy of the network) is conserved. Analogously, all domains of the types B and C can be moved in the two other directions. When a domain is moved by one lattice unit in such a way, the signs of all spins inside it are reversed.

A combination of all three types of zero modes allows to change the size of a three-domain complex (a bubble) formed by neighboring domains of three different types without changing its position. An example of such a bubble is shown in Fig. 7 by the bold line. The zero modes of this particular type are called the breathing modes.<sup>36</sup>

The existence of breathing modes has been discovered by Villain<sup>34</sup> when studying the formation of a honeycomb network in which each domain has the shape of a hexagon. In such a network the size of each hexagon can be changed without changing the total length of domain walls. A honeycomb network is formed in a system with a threefold degeneracy in which a domain wall of a given type (for example, a wall between A and B) can have only three particular orientations out of six that are generally allowed. In these terms, in our problem a wall of each type can have only two orientations out of six, whereas in the three-state Potts model on a triangular lattice all six orientations are allowed for domain walls of any type.

The entropy which can be associated with the existence of zero modes can be estimated as  $\ln M$  per mode, where  $M$  is the typical number of the configurations which can be spanned by a given zero mode. It is clear that in a diluted network  $M$  has to be proportional to  $L$ , the typical distance between the centers of neighboring bubbles (in lattice units). This allows one to estimate the free energy (per unit area) of a network shown in Fig. 7 as

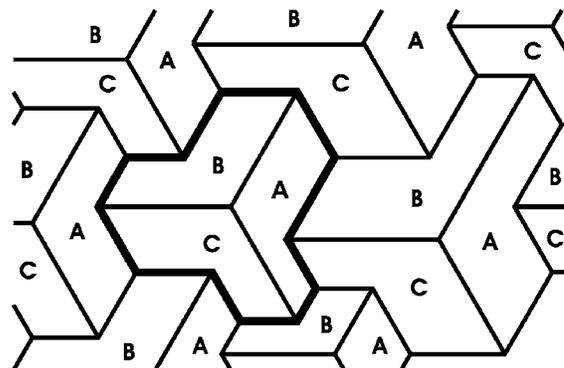


FIG. 7. A possible structure of a domain-wall network.

$$F_{\text{nw}}(L) \approx \frac{2}{\sqrt{3}} \left[ 4 \frac{E_{\text{dw}}}{L} + 3 \frac{E_{\text{mp}}}{L^2} - 3T \frac{\ln L}{L^2} + O\left(\frac{1}{L^3}\right) \right], \quad (9)$$

where

$$E_{\text{mp}} = E_a + E_b = 4J_3.$$

The first term in the right-hand side of Eq. (9) describes the energy of domain walls, the second term—the energy of merging points and the third term is related to the entropy of zero modes. The expression (9) has the same structure as the one proposed by Villain<sup>34,35</sup> for a honeycomb network.

The variation of  $F_{\text{nw}}(L)$  with respect to  $L$  reveals that this function has two minima, one of which is situated at  $L=\infty$  and corresponds to the absence of any network and another at  $L=L_0<\infty$ . The free energies of these two minima become equal to each other when

$$L_0 = \frac{3T}{4E_{\text{dw}}}, \quad \ln L_0 = 1 + \frac{E_{\text{mp}}}{T}. \quad (10)$$

This shows that the applicability of Eq. (9), which assumes  $L \gg 1$ , requires to have  $E_{\text{dw}} \ll T \ll E_{\text{mp}}$ , that is  $E_{\text{dw}} \ll J_2$ . With the increase of  $E_{\text{dw}}/J_2$  the value of  $L_0$  at the transition is decreased and for  $E_{\text{dw}} \sim J_2$  it becomes comparable with 1, which means that Eq. (9) is no longer applicable.

In the limit of  $E_{\text{dw}} \ll J_2$  (when  $E_{\text{mp}} \approx 2J_2$ ) the temperature of the first-order phase transition related to the formation of a domain-wall network, which follows from Eqs. (10), can be estimated as

$$T_{\text{nw}} \approx \frac{E_{\text{mp}}}{\ln(E_{\text{mp}}/E_{\text{dw}})} \approx \frac{2J_2}{\ln(J_2/E_{\text{dw}})}, \quad (11)$$

whereas the value of  $L_0$  (which determines the correlation radius for the fluctuations of  $\sigma_j$ ) at the transition point is given by

$$L_c \approx \frac{3}{2} \frac{J_2/E_{\text{dw}}}{\ln(J_2/E_{\text{dw}})}. \quad (12)$$

With the decrease of  $J_3$  the ratio  $E_{\text{mp}}/E_{\text{dw}}$  is decreased, which leads to the decrease of  $L_c$ . For  $J_3 \sim J_2$  (that is  $E_{\text{dw}} \sim E_{\text{mp}}$ ) the value of  $L_c$  following from Eqs. (10) becomes comparable with 1, which means that the approach based on the minimization of  $F_{\text{nw}}(L)$  is no longer applicable. However, since the decrease of  $J_3$  makes the first-order nature of the transition more and more pronounced, one can expect that it will remain of the first order even when the formation of a domain-wall network does not allow for a quantitative description. In the next section this conclusion is confirmed with the help of a phenomenological analysis which does not take into account any details of a domain-wall network structure and, therefore, is applicable in a wide interval of the values of  $J_3$  (including  $J_3=0$ ).

The finiteness of  $J_1$  cannot be expected to be of any importance for the phase transition related with the spontaneous formation of a domain-wall network. It allows for fluctuations of single domain walls, which no longer have to be straight, but, as has been shown by Villain<sup>35</sup> for a hexagonal network, this does not lead to any qualitative changes.

## V. HIGH-TEMPERATURE PHENOMENOLOGY

Like above, it will be convenient to start the analysis by considering the case of  $J_1=\infty$ . In this limit the manifold of the allowed states coincides with the manifold of the ground states of the system with only nearest neighbor interaction, which can be put into correspondence with the states of the (111) facet of a crystal with a simple cubic lattice.<sup>6</sup>

In particular, the ground states whose structure is shown in Fig. 1 map onto the states with the maximal possible slope, corresponding to the transformation of the (111) facet into one of the three facets of the (100) family. The direction of the slope is determined by the direction of stripes in spin representation. These states do not allow for the formation of any finite size defects, because this would require locally the further increase of a slope.

In the limit of  $T \rightarrow \infty$  all terms in the partition function become equal to each other, therefore in this limit all correlation functions in the system with  $J_1=\infty$  have exactly the same form as in the model with the interaction of only nearest neighbors at zero temperature. The corresponding phase is characterized by the zero slope and a logarithmical divergence of fluctuations<sup>6</sup> of the discrete variable  $n$  describing the position of a surface. One can expect that the same phase will be also stable at large but finite  $T$ .

In this phase the large-scale fluctuations of  $n$  can be described by a continuous free energy functional,

$$F_{\text{eff}}\{n\} = \int d^2\mathbf{r} f_2\{n\}, \quad f_2\{n\} = \frac{K}{2} (\nabla n)^2, \quad (13)$$

in which the discreteness of  $n$  is neglected.<sup>6</sup> At  $T=\infty$  the dimensionless effective rigidity  $K$  (which is of entropic origin) is equal to  $K_0=\pi/9$ . In terms of the SOS representation the energy of a step (per unit length) is equal to  $-2J_2$ , therefore, for  $J_2<0$  the decrease of temperature is accompanied by a monotonic growth of  $K$ ,<sup>9</sup> which at  $K=\pi/2$  leads to the phase transition to the smooth phase.

We are now considering the opposite case of  $J_2>0$ , when the decrease of  $T$  from  $T=\infty$  should be accompanied by the decrease of  $K$  from  $K=K_0$ . Since we know that at lower temperatures the triply degenerate phase with a finite slope has to be formed, the phenomenological functional (13) has to be replaced by a more complex one,

$$F_{\text{eff}}\{n\} = \int d^2\mathbf{r} (f_2\{n\} + f_3\{n\} + f_4\{n\}), \quad (14)$$

where the second term in the integrand,

$$f_3\{n\} = -K_3 [(\mathbf{e}_1 \nabla n)][(\mathbf{e}_2 \nabla n)][(\mathbf{e}_3 \nabla n)], \quad (15)$$

favors a finite slope in one of the three equivalent directions set by the three unit vectors  $\mathbf{e}_\alpha$  (where  $\alpha=1, 2, 3$ ) forming the angles of  $120^\circ$  with each other. The last term in the integrand,  $f_4\{n\}$ , is required to stabilize a finite value of a slope. On general grounds, one can expect that the expansion of  $f_4\{n\}$  in powers of  $\nabla n$  starts from the fourth-order contribution:

$$f_4\{n\} = \frac{K_4}{4} (\nabla n)^4 + \dots \quad (16)$$

Note that the free energy functional (14) has nothing in common with the Ginzburg-Landau functional constructed by Domany *et al.*<sup>16</sup> In particular, in the latter the third-order term can appear only in the absence of the particle-hole symmetry (which in terms of the spin representation corresponds to  $s_j \Rightarrow -s_j$ ). In the model that we consider this symmetry is, naturally, always present, but  $F_{\text{eff}}\{n\}$  has to contain the third-order term just as a consequence of the symmetry of the problem in terms of the SOS representation.

From the form of  $F_{\text{eff}}\{n\}$  it is clear that a phase transition between the phases with zero and finite slopes cannot occur in a continuous way. The three equivalent auxiliary minima of  $F_{\text{eff}}\{n\}$  are formed at finite values of  $|\nabla n|$ , and a first-order phase transition takes place when the decrease of  $K$  makes the free energy in these minima lower than in the central minimum at  $|\nabla n|=0$ .

Thus we have obtained an additional confirmation of the conclusion that a phase transition from the disordered phase with a zero slope to a phase with a finite slope has to be of the first order. Naturally, the construction of a phenomenological functional does not allow one to distinguish whether it has to be a direct transition to the completely frozen phase with the maximal possible slope, or a transition to an intermediate phase with a smaller slope (that is, with a finite concentration of spontaneously formed double domain walls), which at lower temperatures will be followed by the second phase transition.

At finite  $J_1$  the height variable  $n$  can no longer be uniquely defined. In terms of  $n$  each plaquette at which the condition (2) is violated corresponds to a screw dislocation on going around which  $n$  changes by  $\pm 6$ .<sup>9</sup> The core energy of such dislocations is close to  $2J_1$ , whereas their logarithmic interaction is too weak to keep them bound in pairs.<sup>9</sup> In such a situation the effective free energy should be a functional not of a multivalued variable  $n$ , but of its derivatives,

$$m_\alpha = (\mathbf{e}_\alpha \nabla) n,$$

which in the presence of free dislocations do not have to satisfy the condition

$$m_1 + m_2 + m_3 = 0. \quad (17)$$

This can be taken into account by making in Eqs. (13)–(16) a replacement,

$$(\nabla n)^2 \Rightarrow \frac{2}{3}(m_1^2 + m_2^2 + m_3^2), \quad (\mathbf{e}_\alpha \nabla) n \Rightarrow m_\alpha,$$

and adding to it a new contribution,

$$f_D = \frac{K_D}{2}(m_1 + m_2 + m_3)^2$$

(where  $\ln K_D \propto 2J_1/T$ ), which controls the fluctuations of the difference between the densities of positive and negative dislocations. However, the minimums of this new functional, which instead of the two variables encoded in  $\nabla n$  depends on the three variables  $m_\alpha$ , will be achieved when they satisfy the condition (17), and therefore, the conclusion on the first order of the transition (obtained at  $J_1 = \infty$ ) will hold also at large but finite  $J_1$ .

## VI. COMPARISON OF DIFFERENT SCENARIOS OF DISORDERING

In the two previous sections we have demonstrated that the phase transition to the completely disordered phase (which can be associated with the formation of a network of single domain walls) has to be of the first order. This still leaves possibilities for two different scenarios of disordering. The formation of a network of domain walls can either happen at  $T = T_{\text{nw}} > T_2$  as a separate phase transition, or at  $T_{\text{nw}} \leq T_2$ . In the latter case at  $T > T_{\text{nw}}$  the system is already in the disordered phase (in which the domains of all six ground states are intermixed with each other) and nothing special can be expected to happen at  $T = T_2$ . In that case the only phase transition takes place at  $T = T_{\text{nw}}$ .

In the Appendix we demonstrate how at  $J_1 = \infty$  one can construct  $T_c^+$ , an exact upper boundary for  $T_c$ , the temperature of a phase transition from the completely frozen phase,  $T_c = \min\{T_2, T_{\text{nw}}\}$ . The expression we obtain, Eq. (A2), is applicable for an arbitrary relation between  $J_2$  and  $J_3$ . In the case  $J_3 = 0$  it gives  $T_c^+ \approx 7.54J$ , which is only 6% above the value of  $T_2(J_3 = 0) = \gamma_2 T_2$  discussed in Sec. III. Since there are no reasons for this boundary from above to give an extremely accurate estimate of  $T_c$ , one can expect that the real value of the temperature at which the fluctuations on the background of the completely frozen phase do appear will be even lower than  $T_2$ , which means that for  $J_3 = 0$  the single-transition scenario is realized.

Comparison of Eq. (8) with Eq. (11) shows that in the region of parameters in which one can rather accurately estimate both  $T_2$  and  $T_{\text{nw}}$ , these two temperatures coincide with each other with the logarithmical accuracy. This gives a hint that both mechanisms may be different manifestations of the same phenomenon.

This idea looks even more plausible when one notices that the fluctuations of a double domain wall considered in Sec. III can also be discussed in terms of zero modes. That is, the parallelogram in the middle of Fig. 4(b) also can be considered as a domain which can be moved along the direction of domain walls that are adjacent to it without changing the total length of the walls. Apparently, a typical network will have a less regular structure than the network shown in Fig. 7 and will incorporate some fragments looking like finite pieces of a double wall. However, the contribution to the free energy from each zero mode has to be of the form

$$cE_{\text{dw}}L + (E_a + E_b) - T \ln L,$$

where  $c \sim 1$ , which after summation over all modes will reproduce the general structure of Eq. (9). This suggests that there should be only one phase transition which is of the first order and is related to the appearance of a network formed both by single and double domain walls.

Comparison of Eq. (8) with Eq. (11) shows that the realization of the two-transition scenario with  $T_2 < T_{\text{nw}}$  requires  $E_c \leq E_{\text{mp}}$ . When only  $J_1$ ,  $J_2$ , and  $J_3$  are assumed to be non-zero,  $E_c$  satisfies the relation

$$E_c = E_a + E_b + E_{dw} > E_{mp},$$

and, therefore, any prerequisites for the phase transition splitting are absent. Nonetheless, they may appear when one takes into account the interaction of more distant neighbors.

In particular, if one includes into consideration the interaction of fifth neighbors (see Fig. 2), it turns out that  $E_{dw}$ ,  $E_{ddw}$ , and  $E_c$  remain unchanged, and therefore,  $T_2$  should not depend on  $J_5$ . On the other hand,  $E_{mp}$  is increased by  $8J_5$ , which according to Eq. (11) will shift the value of  $T_{nw}$  upwards. Thus, one can expect that the increase of  $J_5$  will lead to the splitting of the phase transition into two.

However, the positiveness of  $J_4$  works in the opposite direction and therefore in a realistic system in which the coupling constants continuously depend on the distance between sites, the influence of  $J_5$  is likely to be compensated by the influence of  $J_4$  (unless  $J_4$  is, for some reasons, of the opposite sign). Nonetheless, the possibility of phase transition splitting is not entirely prohibited, although its realization in some physical system is not very probable.

## VII. CONCLUSION

In the present work we have investigated the scenarios of disordering of the striped phase which is formed in a triangular-lattice Ising model with the antiferromagnetic interaction of nearest and next-to-nearest neighbors. Our analysis has shown that the destruction of such an ordering has to take place via a single first-order phase transition.

The nature of this transition becomes more transparent in the case  $J_2 - 2J_3 \ll J_2$ , when it can be discussed in terms of the formation of a *diluted* network of domain walls, which is characterized by an extensive number of zero modes. In this limit one can find how the transition temperature and the value of the correlation radius at the transition point depend on the parameters of the model [see Eqs. (11) and (12)]. In the opposite limit of  $J_3 \rightarrow 0$  the transition temperature has to be proportional to  $J_2$ , the only energy scale which is relevant for  $J_2 \ll J_1$ , whereas the correlation radius at the transition point has to be comparable with 1.

We also have shown that the formation of a domain-wall network could be anticipated by a transition to the intermediate phase, in which the long-range order in terms of  $\sigma_j$  is destroyed by the spontaneous formation of a sequence of parallel (on the average) double domain walls, whereas the long-range order in the orientation of stripes formed by the spins of the same sign still exists. This transition would be characterized by a combination of the Ising (in the very narrow vicinity of the transition temperature) and the Pokrovsky-Talapov (in a more wide temperature interval) critical behaviors. However, in a system with only three coupling constants ( $J_1$ ,  $J_2$ , and  $J_3$ ) no prerequisites for the realization of such a scenario can be found.

Nonetheless, they may appear when the interaction of more distant neighbors is taken into account. In particular, the splitting of the phase transition into two is favored by the increase of  $J_5$ . However, the possibility of the realization of such a scenario depends on the fine interplay between different coupling constants  $J_k$  with  $k \geq 4$  and in a system with a

monotonic dependence of  $J_k$  on  $k$  is not very probable.

An additional mechanism favoring the two-transition scenario may be related to quantum fluctuations, whose role in decreasing the energy of double walls may be more prominent than in decreasing the energy of a diluted network due to a smaller size of moving objects in the former case.

The numerical simulations of the triangular-lattice Ising antiferromagnet have been performed in Refs. 25–28. In particular, Glosli and Plischke<sup>25</sup> have studied the system with first and second neighbor interactions satisfying  $J_2/J_1=0.1$ , Rastelli *et al.*<sup>27</sup>—with  $J_2/J_1=0.1, 0.5, 1$ , whereas Novikov *et al.*<sup>26</sup> have assumed that the interaction decays with the distance exponentially. The results of these groups give evidence for the existence of a single first-order transition, which is consistent with our conclusions. In the simulations of Takagi and Mekata<sup>28</sup> the disordering of the striped phase has been investigated in the system with  $J_2/J_1=0.2$  or  $0.5$  and  $J_3/J_1=-0.75$ , but these authors make no conclusions about the type of the phase transition which they observe.

In addition to more traditional applications mentioned in the Introduction, the considered version of the Ising model can be used for the description of a triangular array of quantum dots at half-filling<sup>26</sup> and (at sufficiently low temperatures) of a Josephson junction array with the dice lattice geometry and one-third of the flux quanta per plaquette.<sup>39</sup> In the latter case the role of  $J_k$  with  $k > 1$  is played by the magnetic interactions of currents in the array.<sup>39,40</sup> The results of this work may also be of help for understanding the nature of phase transition(s) in the fully frustrated XY model on a honeycomb lattice,<sup>41,42</sup> in which the fluctuation-induced vortex pattern<sup>42</sup> has the same structure as in Fig. 1.

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## APPENDIX: AN EXACT UPPER BOUNDARY FOR $T_c$ IN THE LIMIT $J_1 \rightarrow \infty$

In the limit  $J_1 \rightarrow \infty$  it is convenient to split the Hamiltonian (1) into two terms,

$$H = H_0 + (H - H_0),$$

the first of which,  $H_0$ , includes only the infinite interaction of nearest neighbors and restricts the summation in the partition function to the states in which the constraint (2) is satisfied on all triangular plaquettes, whereas the second term,  $H - H_0$ , includes all other interactions. It is well known<sup>43</sup> that the application of a variational procedure allows one to use such a splitting to demonstrate that the free energy of the system,  $F$ , is bounded from above by

$$F^+ \equiv F_0 + \langle H - H_0 \rangle_0, \quad (\text{A1})$$

where  $F_0$  is the free energy of the system whose Hamiltonian is equal to  $H_0$ , whereas the angular brackets denote the average calculated with the help of  $H_0$ .

In our case in the thermodynamic limit

$$F_0 = -N(J_1 + Ts_0),$$

$$\langle H - H_0 \rangle_0 = 3N(J_2 g_2 + J_3 g_3),$$

where  $N$  is the total number of sites,

$$s_0 \approx 0.323066$$

is the residual entropy,<sup>2</sup> whereas  $g_k = \langle \sigma_i \sigma_j \rangle_0$  is the correlation function of the variables  $\sigma$  on the sites  $\mathbf{i}$  and  $\mathbf{j}$  which are the  $k$ th neighbors of each other, calculated for the system with only nearest neighbor interaction at  $T=0$ . According to Stephenson<sup>4</sup>

$$g_2 = \frac{1}{9} + \frac{2}{\sqrt{3}\pi}, \quad g_3 = \frac{1}{9} - \frac{3}{\pi^2}.$$

The comparison of  $F^+(T)$  with the free energy of a completely frozen ground state, which, naturally, coincides with its energy,

$$E_0 = -N(J_1 + J_2 - 3J_3),$$

allows one to conclude that the temperature  $T_c$ , at which a phase transition from a completely frozen state to some

phase with more developed fluctuations takes place, cannot be larger than

$$T_c^+(J_2, J_3) = C_2 J_2 - C_3 J_3, \quad (\text{A2})$$

where

$$C_2 = (1 + 3g_2)/s_0 \approx 7.54, \quad (\text{A3})$$

$$C_3 = 3(1 - g_3)/s_0 \approx 11.08. \quad (\text{A4})$$

Naturally, this approach does not allow to distinguish if the phase transition at  $T=T_c < T_c^+$  is a direct transition into the disordered phase or a transition to the intermediate phase in the framework of a two-transition scenario.

For  $J_3=0$  the value of  $T_c^+$  following from Eqs. (A2) and (A3) is rather close to  $T_2$ , the temperature of the spontaneous formation of double domain walls given by Eq. (7), whereas in the limit of  $E_{dw} \rightarrow 0$  (that is  $J_3 \rightarrow J_2/2$ ) one gets

$$T_c^+ \approx 2.00J_2,$$

which is compatible with an estimate for the temperature of the phase transition given by Eqs. (8) and (11).

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