

Phase transitions in the antiferromagnetic XY model with a *kagomé* lattice

S. E. Korshunov

L.D. Landau Institute for Theoretical Physics, Kosygina 2, Moscow 117940, Russia

(Received 15 June 2001; published 9 January 2002)

The ground state of the antiferromagnetic XY model with a *kagomé* lattice is known to be characterized by a well developed accidental degeneracy. As a consequence the phase transition in this system consists in unbinding of pairs of fractional vortices. Addition of the next-to-nearest neighbor (NNN) interaction leads to stabilization of the long-range order in chirality (or staggered chirality). We show that the phase transition, related with destruction of this long-range order, can happen as a separate phase transition below the temperature of the fractional vortex pairs unbinding only if the NNN coupling is extremely weak, and find how the temperature of this transition depends on coupling constants. We also demonstrate that the antiferromagnetic ordering of chiralities and, accordingly, the presence of the second phase transition are induced by the free energy of spin wave fluctuations even in absence of the NNN coupling.

DOI: 10.1103/PhysRevB.65.054416

PACS number(s): 75.10.Hk, 64.60.Cn, 74.80.-g

I. INTRODUCTION

The antiferromagnetic XY model can be defined by the Hamiltonian

$$H = J_1 \sum_{\text{NN}} \cos(\varphi_i - \varphi_j), \quad (1)$$

where $J_1 > 0$ is the coupling constant, φ_i describes the orientation of the classical planar spin $\mathbf{s}_i = (\cos \varphi_i, \sin \varphi_i)$, belonging to the site i of some regular lattice, and the summation is performed over the pairs of nearest neighbors (NN) on this lattice. The ground state of such model on a *kagomé* lattice (Fig. 1) is known to have a huge accidental (that is not related to the symmetry of the Hamiltonian) degeneracy.¹

For $J_1 > 0$ the minimum of the energy of each triangular plaquette is achieved when the three spins belonging to it form the angles $\pm 2\pi/3$ with each other. In addition to the possibility of a simultaneous rotation of all three spins such arrangement is also characterized by the two-fold discrete degeneracy. When on going clockwise around the plaquette the spins rotate clockwise (anticlockwise), the plaquette can be ascribed the positive (negative) chirality $\sigma = \pm 1$. In the ground state of the antiferromagnetic XY model with triangular lattice the plaquettes with positive and negative chiralities regularly alternate with each other.²

In any ground state on a *kagomé* lattice the variables φ_i analogously acquire only three values which differ from each other by $2\pi/3$. However, the requirements for the arrangement of chiralities are less rigid than on triangular lattice and accordingly the ground state in addition to the continuous $U(1)$ degeneracy (related with an arbitrary simultaneous rotation of all spins) is characterized by a well developed discrete degeneracy (of the same type as in the 3-state antiferromagnetic Potts model) leading to a finite residual entropy per site.^{1,3}

The accidental degeneracy persists if the interaction function in Eq. (1) differs from the pure cosine (remaining even), but is removed by the presence of interactions with more

distant neighbors. In particular, for the ferromagnetic sign ($J_2 < 0$) of the next-to-nearest neighbors (NNN) interaction the minimum of

$$H_2 = J_1 \sum_{\text{NN}} \cos(\varphi_i - \varphi_j) + J_2 \sum_{\text{NNN}} \cos(\varphi_i - \varphi_j) \quad (2)$$

is achieved in one of the so-called $\sqrt{3} \times \sqrt{3}$ states⁴ with a regular alternation of positive and negative chiralities. An example of such state is shown in Fig. 2(a). Here and further on we use the letters A, B and C to denote three values of φ_i which differ from each other by $\pm 2\pi/3$ (for definiteness let us assume $\varphi_B = \varphi_A + 2\pi/3$, $\varphi_C = \varphi_A + 4\pi/3$). This state has the same structure as the ground state of a planar antiferromagnet with triangular lattice (or, to put it more accurately, can be obtained by the natural truncation of it). On the other hand the NNN interaction of the opposite sign ($J_2 > 0$) favors the ferromagnetic arrangements of chiralities, which is achieved in the so-called $\mathbf{q} = 0$ states,⁴ see Fig. 2(b).

For both signs of the NNN interaction the degeneracy of the ground state is reduced to $U(1) \times Z_2$.⁵ This suggests the possibility of the two phase transitions, one of which is associated with unbinding of vortex pairs [the Berezinskii–Kosterlitz–Thouless (BKT) transition^{6–9}] and the other with proliferation of the Ising type domain walls. The number of the systems with the same degeneracy of the ground state includes, in particular, the antiferromagnetic XY model with triangular lattice^{2,10} and the fully frustrated XY model with square lattice.^{11,12}

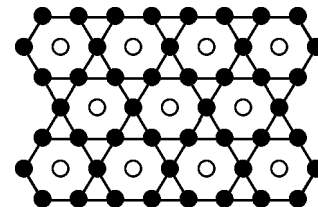


FIG. 1. A *kagomé* lattice (shown by filled circles) can be constructed by the regular elimination of one quarter of sites from a triangular lattice. It consists of triangular and hexagonal plaquettes.

For the case of weak NNN interaction ($|J_2| \ll J_1$) the energy of a domain wall (per unit length) is proportional to $|J_2|$ and the logarithmic interaction of vortices to J_1 . If domain walls and vortices were completely independent one would then expect the phase transition related with breaking of the discrete symmetry group to take place at lower temperature than the BKT transition.

In the present work we analyze the mutual influence between different classes of topological excitations in the antiferromagnetic XY model with a *kagomé* lattice and weak NNN interaction and demonstrate that the phase transition related with the domain walls proliferation (i) can happen as a separate phase transition only for extremely weak NNN interaction, (ii) is not of the Ising type and (iii) the temperature of this transition is *not* proportional to the strength of the NNN interaction as one could naively expect. We also show that at very low temperatures the free energy of spin waves leads to stabilization of the antiferromagnetic ordering of chiralities even in absence of the NNN interaction.

The results can be of interest in relation with possible presence of weak easy-plane anisotropy in Heisenberg *kagomé* antiferromagnets,¹³ which is indirectly confirmed by recent investigations of susceptibility¹⁴ in $(\text{H}_3\text{O})\text{Fe}_3(\text{SO}_4)_2(\text{OH})_6$. The other class of physical systems, which allows for experimental realization of the considered model, consists of Josephson junction arrays¹⁵ and two-dimensional superconducting wire networks¹⁶ in perpendicular magnetic field. In such systems the role of φ_i is played by the phase of the superconducting order parameter, and equivalence with the antiferromagnetic XY model is achieved when the magnitude of the magnetic field corresponds to half-integer number of superconducting flux quanta per each triangular plaquette. A superconducting array, which can be described by the same model in absence of the external magnetic field, can be constructed with the help of so-called π -junctions.¹⁷

II. ZERO TEMPERATURE: THE EQUIVALENT SOLID-ON-SOLID MODEL

It has been already mentioned in the Introduction that the set of the ground states of the Hamiltonian (1) is equivalent (up to a simultaneous rotation of all spins) to that of the 3-state antiferromagnetic Potts model.^{1,3} Any triangular plaquette of a *kagomé* lattice has to contain some permuta-

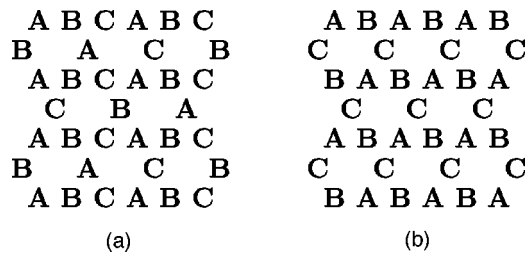


FIG. 2. The structure of the ground states selected in presence of interactions with further neighbors. The letters A, B and C correspond to the three values of φ_i , which differ from each other by $\pm 2\pi/3$. (a) A $\sqrt{3} \times \sqrt{3}$ state; (b) a $\mathbf{q}=0$ state.

tion of the three values of φ_i (φ_A , φ_B and φ_C), which can be identified with the three states ($\alpha=1,2,3$) of the antiferromagnetic Potts model.

The degeneracy of such set of ground states can be discussed in terms of the zero-energy domain walls. If one considers a $\sqrt{3} \times \sqrt{3}$ ground state [Fig. 2(a)], it turns out possible to construct the state with the same energy by permutation (for example) of the form $\varphi_B \leftrightarrow \varphi_C$ inside any closed loop formed by the sites with $\varphi_i = \varphi_A$, etc. Such closed loop [a simplest example of which is shown in Fig. 3(a)] can be considered as the zero-energy domain wall separating two different $\sqrt{3} \times \sqrt{3}$ states with the opposite signs of staggered chirality. Any domain wall with zero energy is formed by elementary links which have to join each other at the angles of $\pm 2\pi/3$ [Fig. 3(b)]. Each link separates two triangular plaquettes with the same chirality, that is with the opposite signs of staggered chirality. The states with infinite (un-closed) domain walls are also possible.

There exists¹⁸ the exact mapping of the set of the ground states of the 3-state antiferromagnetic Potts model onto the states of the solid-on-solid (SOS) model in which the “height” variables $\mathbf{u}(\mathbf{r})$ are defined on the sites \mathbf{r} situated at the centers of hexagonal plaquettes of a *kagomé* lattice. These sites are shown in Fig. 1 by empty circles. They form the triangular lattice we shall denote \mathcal{T} . Each site of the *kagomé* lattice can be associated with some bond $\mathbf{r}\mathbf{r}'$ of \mathcal{T} and each variable $\varphi_i = \varphi_A, \varphi_B, \varphi_C$ with the Potts variable $\alpha(\mathbf{r}\mathbf{r}') \equiv \alpha(\mathbf{r}'\mathbf{r})$ defined on this bond.

Since each triangular plaquette of a *kagomé* lattice should always contain three different variables φ_A , φ_B and φ_C , one can associate them with three basic vectors \mathbf{a}_α ($\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3 = 0$, see Fig. 4) of some auxiliary triangular lat-

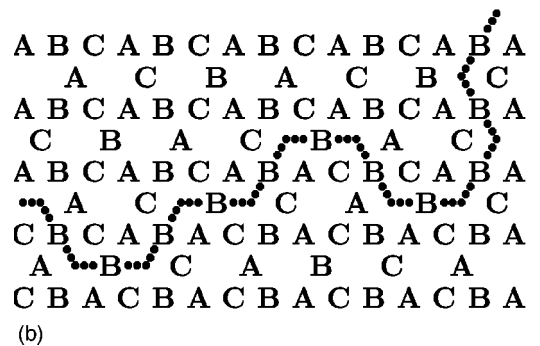
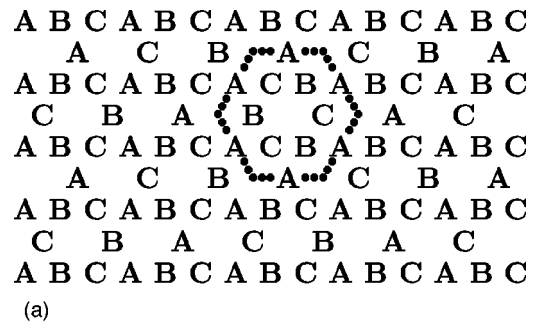


FIG. 3. Two examples of a domain wall separating different $\sqrt{3} \times \sqrt{3}$ states.

tice, which we shall denote \mathcal{T}_a ($a=|\mathbf{a}_\alpha|$ being its lattice constant). The height variables $\mathbf{u}(\mathbf{r})$, which acquire the values $\mathbf{u} \in \mathcal{T}_a$, can be then introduced following the rule

$$\mathbf{u}(\mathbf{r}') = \begin{cases} \mathbf{u}(\mathbf{r}) + \mathbf{a}_{\alpha(\mathbf{r}\mathbf{r}')} & \text{for } \mathbf{r}' = \mathbf{r} + \mathbf{e}_\alpha \\ \mathbf{u}(\mathbf{r}) - \mathbf{a}_{\alpha(\mathbf{r}\mathbf{r}')} & \text{for } \mathbf{r}' = \mathbf{r} - \mathbf{e}_\alpha, \end{cases} \quad (3)$$

where \mathbf{e}_α are the three basic vectors of \mathcal{T} ($\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3 = 0$), as soon as the value of $\mathbf{u}(\mathbf{r}_0)$ is chosen for an arbitrary site \mathbf{r}_0 .¹⁸

This defines the correspondence between the states of the antiferromagnetic Potts model and of the ‘‘vector’’ SOS model, in which the height variables $\mathbf{u}(\mathbf{r}) \in \mathcal{T}_a$ have to satisfy the constraint

$$|\mathbf{u}(\mathbf{r}) - \mathbf{u}(\mathbf{r}')| = a \quad (4)$$

on all pairs of neighboring sites of \mathcal{T} . By using the known properties of the exact solution¹⁹ of the 3-state antiferromagnetic Potts model with external field coupled to staggered chirality Huse and Rutenberg¹ have demonstrated (and also have confirmed this conclusion by numerical calculation) that such vector SOS model, in the partition function of which all allowed configurations of heights are counted with the same weight, is situated exactly at the point of the roughening transition, where (for $|\mathbf{r}_1 - \mathbf{r}_2| \gg 1$)

$$\langle [|\mathbf{u}(\mathbf{r}_1) - \mathbf{u}(\mathbf{r}_2)|]^2 \rangle \approx \frac{3a^2}{\pi^2} \ln |\mathbf{u}(\mathbf{r}_1) - \mathbf{u}(\mathbf{r}_2)|. \quad (5)$$

Therefore any additional perturbation suppressing the fluctuations will lead to transition of the system into the flat phase, in which the fluctuations of \mathbf{u} are convergent.

According to constraint (4) the variables $\mathbf{u}(\mathbf{r})$ on neighboring sites have to be different from each other, so that even the most flat state is formed by the regular alternation of three different values of \mathbf{u} . The transition into the flat phase can be more transparently discussed in terms of the variables

$$\mathbf{n}(\mathbf{R}) \equiv \frac{\mathbf{u}(\mathbf{r}) + \mathbf{u}(\mathbf{r}') + \mathbf{u}(\mathbf{r}'')}{3} \quad (6)$$

describing the average height at each of the plaquettes of \mathcal{T} . The variables $\mathbf{n}(\mathbf{R})$ are defined at the sites \mathbf{R} of the honeycomb lattice \mathcal{H} , which is dual to \mathcal{T} , and acquire the values $\mathbf{n}(\mathbf{R}) \in \mathcal{H}_a$, where \mathcal{H}_a is the honeycomb lattice which is dual to \mathcal{T}_a (Fig. 4). In terms of the original spin variables the flat states [in which all variables $\mathbf{n}(\mathbf{R})$ are equal to each other]

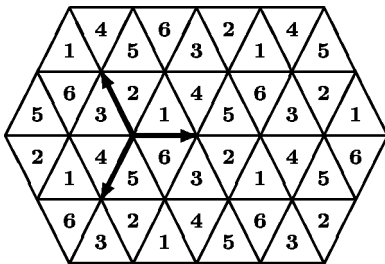


FIG. 4. The triangular lattice \mathcal{T}_a and its three basic vectors \mathbf{a}_α . The sites of the dual lattice \mathcal{H}_a are shown by the numbers from 1 to 6. The same numbers correspond to physically equivalent states.

correspond to $\sqrt{3} \times \sqrt{3}$ states, and zero-energy steps, the presence of which leads to their roughening, to the zero-energy domain walls separating different $\sqrt{3} \times \sqrt{3}$ states.

The large scale properties of the vector SOS model introduced above (and of its further generalizations) can be analyzed with the help of the multi-component sine-Gordon model with the same symmetry. The (dimensionless) Hamiltonian of such sine-Gordon model can be chosen in the form

$$H_{\text{SG}} = \int d^2\mathbf{R} \left\{ \frac{KQ^2}{2} [\nabla \mathbf{n}(\mathbf{R})]^2 + y \sum_{\alpha=1}^3 \cos[\mathbf{Q}_\alpha \mathbf{n}(\mathbf{R})] \right\}. \quad (7)$$

The first term in Eq. (7) describes the effective stiffness (of entropic origin) which can be associated with the fluctuations of $\mathbf{n}(\mathbf{R})$, whereas the second term favors the values of $\mathbf{n}(\mathbf{R})$ which belong to \mathcal{H}_a . Here \mathbf{Q}_α are the three basic vectors of the triangular lattice reciprocal to \mathcal{T}_a , so

$$\mathbf{Q}_\alpha^2 = \frac{16\pi^2}{3a^2}; \quad \mathbf{Q}_1 + \mathbf{Q}_2 + \mathbf{Q}_3 = 0.$$

Analogous Hamiltonian (with the opposite sign of the second term) and equivalent vector Coulomb gas have been investigated by Nelson in relation with dislocation mediated melting in two-dimensional crystals.²⁰ Alternatively the Hamiltonian of the form (7) can be interpreted as a simplified model for pinning of a two-dimensional crystal by a periodic substrate (cf. with Ref. 21). Note, however, that in contrast to real two-dimensional crystals, the accurate description of which requires to distinguish between compression and shear moduli, in our system the displacement \mathbf{n} takes place in some auxiliary space (and not in the real space) and, therefore, only one elastic modulus can be introduced.

The renormalization group equations of Ref. 20, describing the evolution of K and y with the change of the length scale L , in our notation can be rewritten as

$$\frac{dK}{dl} = \frac{3\pi}{8} y^2, \quad (8a)$$

$$\frac{dy}{dl} = \left(2 - \frac{1}{4\pi K} \right) y - \pi y^2, \quad (8b)$$

where $l = \ln L$. The corresponding flow diagram is schematically shown in Fig. 5, where $K_c \equiv 1/(8\pi)$. It suggests that the roughening transition takes place when the renormalized value of the effective stiffness K is equal to K_c . The vector SOS model described above (which is known to be at the point of its roughening transition¹) can therefore be associated with some point belonging to the left separatrix.

III. PHASE TRANSITION(S) ASSOCIATED WITH VORTEX PAIRS UNBINDING

At finite temperature T other types of fluctuations (requiring finite energy) become possible, in particular formation of vortex pairs. Vortices are pointlike topological excitations (the local minima of the Hamiltonian), the existence of

which is related with the multivaluedness of the field φ . On going around each vortex φ experiences a continuous twist which adds to $\pm 2\pi$. At low temperatures all vortices are bound in neutral pairs by their logarithmic interaction.⁷

With increase in temperature this interaction becomes renormalized due to mutual influence of different vortex pairs and becomes screened at the temperature T_{BKT} of the BKT transition,⁷⁻⁹ which leads to dissociation of vortex pairs and exponential decay of correlations of $\exp(i\varphi)$ (in contrast to algebraic decay⁶ at $T < T_{\text{BKT}}$). The value of the helicity modulus Γ , describing the effective stiffness of spin system with respect to infinitely small twist, at the temperature of vortex pairs dissociation is known to satisfy the universal relation:²²

$$T_{\text{BKT}} = \frac{\pi}{2} \Gamma(T_{\text{BKT}}). \quad (9)$$

Huse and Rutenberg¹ have argued that since at $T=0$ the antiferromagnetic XY model with *kagomé* lattice is characterized by the long range order in $\exp(i3\varphi)$ rather than in $\exp(i\varphi)$, the phase transition in this system should consist in unbinding of pairs of fractional vortices with topological charges $\pm 1/3$ and not of the ordinary (integer) vortices. The strength of the logarithmic interaction of fractional vortices is decreased by the factor of 9 in comparison with that of integer vortices,¹³ therefore relation (9) should be replaced by

$$T_{\text{FV}} = \frac{\pi}{18} \Gamma(T_{\text{FV}}), \quad (10)$$

where T_{FV} is the temperature of the phase transition, associated with unbinding of pairs of fractional vortices.

The value of Γ in any ground state of the antiferromagnetic XY model with *kagomé* lattice is equal to $\Gamma_0 = (\sqrt{3}/4)J_1$. Substitution of Γ_0 into Eq. (10) [instead of $\Gamma(T_{\text{FV}})$] allows to obtain for T_{FV} the estimate (from above) of the form

$$T_{\text{FV}} \approx \frac{\pi\sqrt{3}}{72} J_1 \approx 0.075 J_1, \quad (11)$$

which turns out to be in reasonable agreement with the results of numerical simulations by Rzchowski,²³ who by using

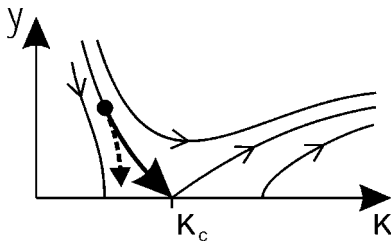


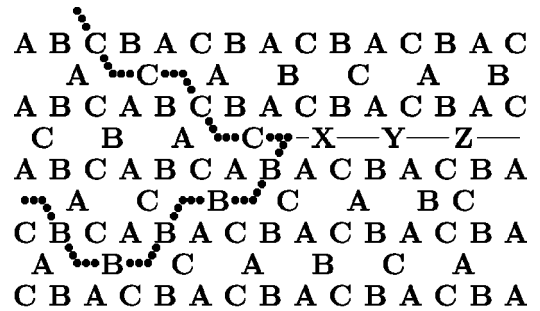
FIG. 5. The schematic flow diagram for Eqs. (8). The system with only NN interaction and $T=0$ can be associated with some point (shown by black dot) on the left separatrix. Dashed arrow shows how the flow is changed at $T>0$ when the contribution from z has to be taken into account.

two different criteria has found $T_{\text{FV}}/J_1 \approx 0.070$ and $T_{\text{FV}}/J_1 \approx 0.076$. In Ref. 24 the same estimate for T_{FV} has been obtained in a less straightforward way with the help of the duality transformation.^{25,26}

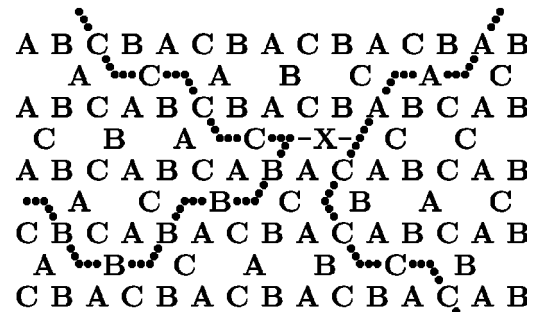
The fractional vortices cannot exist by themselves (in absence of domain walls). A fractional vortex appears at every point where elementary links forming a domain wall meet each other at a wrong angle ($\pi/3$ or π instead of $2\pi/3$). The same happens in the antiferromagnetic XY model with triangular lattice,¹⁰ the ground state of which also has $\sqrt{3} \times \sqrt{3}$ structure. Figure 6(a) shows an example of a domain wall containing one such special point. It separates the domain wall into two segments, one of which is formed by the sites with $\varphi_i = \varphi_C$ and the other by the sites with $\varphi_i = \varphi_B$.

When crossing the first segment the state to the right of the wall should be obtained from the state to the left by the permutation of A and B, whereas for the second segment the state to the right should be obtained by the permutation of A and C. This introduces the discrepancy of $2\pi/3$ which can be localized on a semi-infinite line terminating at the special point (for example on the line X-Y-Z). In order to locally minimize the energy X, Y and Z should be replaced by A, B and C, respectively, when going from above, and by B, C and A when going from below. The misfit of $2\pi/3$ has to be compensated by a continuous twist of φ , which is equivalent to the fractional vortex with the topological charge $-1/3$.

In terms of the vector SOS model each fractional vortex corresponds to the point on going around which the height variable \mathbf{n} changes by $\Delta\mathbf{n}$ with $|\Delta\mathbf{n}| = a$. That means that at each fractional vortex a step with the height $\Delta\mathbf{n}$ (or, to put it more precisely, a set of steps with the total height $\Delta\mathbf{n}$) ter-



(a)



(b)

FIG. 6. (a) An example of a fractional vortex. (b) An example of a dislocation formed by a neutral pair of fractional vortices.

minates or begins. Accordingly the fluctuations of the SOS model provide the additional contribution to the interaction of the fractional vortices related with the difference in entropy between the configurations with different positions of step termination points. At the point of roughening transition of the SOS model, as well as in the rough phase, this additional interaction (which can be expressed in terms of the correlation function of the dual XY model²⁷) is also logarithmic. Its presence shifts T_{FV} upwards and diminishes the mutual influence between fractional and integer vortices. It is known²⁸ that such mechanism in principle can lead to appearance of the separate phase transition, associated with unbinding of pairs of integer vortices, at temperatures above T_{FV} .

On the other hand at finite temperatures the equivalence with the SOS model is no longer exact. One has to remember that the whole multitude of what we describe as flat states of the vector SOS model in terms of the original spin variables corresponds (for given φ_A) to only six different $\sqrt{3} \times \sqrt{3}$ states, which can be obtained from the state shown in Fig. 2(a) by all possible permutations of A, B and C. In Fig. 4 the sites of \mathcal{H}_a , which correspond to equivalent states in terms of φ_i , are designated by the same numbers. In the zero-temperature partition function of the vector SOS model the properties of the zero-energy domain walls separating such states (in particular, two closed loops formed by such walls cannot cross each other but can be situated inside each other or touch each other) allow to count them as different states of the SOS model.^{18,29} At finite temperature it becomes possible for a set of steps separating two physically equivalent states to terminate at the point where all these steps merge together.³⁰ The energy E_D of such defect is finite and proportional to J_1 : $E_D = c_D J_1$, where c_D is of the order of one.

In terms of the multi-component sine-Gordon model (7) such defects correspond to dislocations of the field \mathbf{n} , the (elementary) Burgers vectors of which \mathbf{b}_α ($\alpha=1,2,3$) are given, as can be seen from Fig. 4, by

$$\mathbf{b}_1 = \mathbf{a}_3 - \mathbf{a}_2, \quad \mathbf{b}_2 = \mathbf{a}_1 - \mathbf{a}_3, \quad \mathbf{b}_3 = \mathbf{a}_2 - \mathbf{a}_1. \quad (12)$$

An example of a dislocation is schematically shown in Fig. 6(b). It is formed by a neutral pair of fractional vortices that are sitting on two domain walls which cannot be transformed into a single domain wall. The letter X denotes the site on which $\varphi_i \approx (\varphi_A + \varphi_B)/2$. In the vicinity of this site the values of φ_i slightly deviate from those implied by the letters A, B and C. Successive application of the rule (3) along the perimeter of any closed loop surrounding point X sums up to $\Delta \mathbf{n} = \mathbf{a}_2 - \mathbf{a}_1$.

The renormalization of the dislocation fugacity $z = \exp(-c_D J_1/T)$ with the change of the length scale can be described²¹ by

$$\frac{dz}{dl} = \lambda_z z + 2\pi z^2, \quad (13)$$

where

$$\lambda_z = 2 - \frac{KQ^2 b^2}{4\pi} \equiv 2 - 4\pi K. \quad (14)$$

In the vicinity of the roughening transition ($K \approx K_c$) the exponent λ_z , describing the renormalization of z , is close to $\lambda_z^0 = 3/2$, which corresponds to the fast growth of z . Comparison of λ_z with $\lambda_y = 2 - 1/(4\pi K)$ shows that y and z are never simultaneously irrelevant. In that respect the situation is quite analogous to what is encountered when considering the conventional (ferromagnetic) XY model with weak but relevant (low-order) anisotropy.^{25,31}

The presence of dislocations (or, to put it more accurately, of dislocation pairs) leads also to appearance in the right-hand side of Eq. (8a) of the additional (negative) term proportional to z^2 . The presence of this term shifts the flow (see Fig. 5) from the separatrix to the area which corresponds to the rough phase of the SOS model.

On the other hand the unrestricted growth of z under the renormalization means that the system will contain the finite concentration of free dislocations, which transforms the rough phase of the SOS model into the disordered phase of the six-state model. The decay of correlations in this phase can be characterized by a finite correlation radius ξ_z , which can be found as the length-scale at which z_R (the renormalized value of z) becomes of the order of one. ξ_z defines the scale at which the additional (entropic) interaction of the fractional vortices induced by the fluctuation of the domain walls is screened. The finiteness of ξ_z closes even the hypothetical possibility for dissociation of pairs of integer vortices to take place as a separate phase transition at $T > T_{FV}$.

IV. THE CASE OF THE FERROMAGNETIC NNN INTERACTION

Inclusion into consideration of the interaction with more distant neighbors leads to removal of the accidental degeneracy and stabilizes the states with either ferromagnetic or antiferromagnetic ordering of chiralities of triangular plaquettes.

In the case of the ferromagnetic NNN interaction ($J_2 < 0$) the energy is minimal in one of the $\sqrt{3} \times \sqrt{3}$ states with uniform staggered chirality [Fig. 2(a)]. Figure 3 shows two examples of a domain wall separating two different $\sqrt{3} \times \sqrt{3}$ states with opposite signs of staggered chirality. In the case of only NN interaction such domain wall (consisting of elementary links making angles of $2\pi/3$ with each other) simply costs no energy. The presence of a weak ferromagnetic NNN interaction makes the energy of such domain wall (per elementary link) E_{DW} equal to $-3J_2 > 0$. Here and further on we are interested only in the case $|J_2| \ll J_1$, when the values of the variables φ_i remain close to those shown in Fig. 3 not only away from the wall, but also in the vicinity of the wall.

Note that such wall can fluctuate (make turns, form kinks, etc.) without having to pay the energy proportional to J_1 and, therefore, naively one could expect that the temperature of the phase transition, related with proliferation of such walls and leading to destruction of the long-range order in staggered chirality, should be determined entirely by J_2 . Such conclusion, implicitly based on the comparison of the energy of an infinite domain wall with the negative entropic contribution to its free energy (the Peierls argument³²), does not

take into account that the presence of an infinite domain wall leads also to suppression of the entropy (because it decreases the possibilities for formation of closed domain wall loops) and in some cases does not work.

In Sec. II we have discussed the properties of the vector SOS model to which the antiferromagnetic XY -model with *kagomé* lattice is equivalent at $T=0$. In the partition function of this model all allowed configurations of heights are counted with the same weight. In the case of the analogous model with a finite positive energy of a step (which corresponds to $J_2 < 0$) the same partition function is reproduced in the limit of $T \rightarrow \infty$. For any small but finite ratio $-J_2/T > 0$ the SOS model is shifted from the point of roughening transition into the ordered (flat) phase. On the other hand we also know that at finite temperatures the possibility of dislocation creation tends to shift the same system into the disordered phase. One has to consider the competition of these two effects.

In the vicinity of $K = K_c$ the renormalization equations (8) can be rewritten as

$$\frac{dX}{dl} = Y^2, \quad (15a)$$

$$\frac{dY}{dl} = XY + \alpha Y^2, \quad (15b)$$

where

$$X = 2 \left(1 - \frac{K_c}{K} \right), \quad Y = \frac{1}{\pi \alpha}, \quad \alpha = -\frac{1}{\sqrt{6}}. \quad (16)$$

The solution of Eqs. (15) for arbitrary α allows one to find that the critical behavior of the correlation radius ξ in the vicinity of the transition is given³³ by

$$\ln \xi \propto \left(\frac{K_c}{\Delta K} \right)^{\bar{\nu}}, \quad (17)$$

where ΔK is the deviation from the phase transition. In our problem for $E_{DW} \ll T$ the ratio $\Delta K/K_c$ is proportional to E_{DW}/T .

The case of $\alpha=0$ corresponds to Kosterlitz renormalization group equations⁹ for the standard BKT transition, which give $\bar{\nu}=1/2$. The case of $\alpha = +1/\sqrt{6}$ has been considered by Nelson,²⁰ who has found $\bar{\nu}=2/5$. The solution of the same equations for $\alpha = -1/\sqrt{6}$ gives $\bar{\nu}=3/5$.

If the fugacity of dislocations z is so small that even when growing under renormalization it remains much smaller than one up to $L \sim \xi$ [where the renormalization following Eqs. (15) stops anyway and fluctuations of \mathbf{n} are frozen], the system remains in the ordered (flat) phase of the SOS model, that is in the phase with long-range order in staggered chirality. On the other hand if z_R (the renormalized value of z) manages to become of the order of one when the renormalized value of y is still small, the system finds itself in the disordered phase. The estimate for the temperature T_{DW} of the phase transition separating these two regimes (and asso-

ciated with the proliferation of domain walls) can be obtained from the relation $z_R(\xi) \sim 1$, which is equivalent to

$$\ln(1/z) \sim \lambda_z^0 \ln \xi. \quad (18)$$

In our problem

$$\ln(1/z) = c_D J_1 / T \quad (19)$$

and

$$\ln \xi \sim \left(\frac{T}{E_{DW}} \right)^{\bar{\nu}}, \quad (20)$$

which leads to

$$T_{DW} \sim \left(\frac{E_{DW}}{J_1} \right)^{\frac{\bar{\nu}}{1+\bar{\nu}}} J_1 \propto |J_2|^{3/8} J_1^{5/8}. \quad (21)$$

Away from the critical region the behavior of ξ can be described with the help of the self-consistent harmonic approximation,³⁴ which gives $\bar{\nu} = \bar{\nu}_0 = 1$. That means that with increase of $|J_2|/J_1$ the dependence (21) is replaced by $T_{DW} \propto |J_2|^{1/2} J_1^{1/2}$.

Note that the analysis which has led to Eq. (21) has been based on the assumption that all fractional vortices are bound in pairs, and, accordingly, is valid only for $T_{DW} < T_{FV}$. On the other hand the pairs of fractional vortices cannot dissociate at temperatures lower than T_{DW} , because for $T < T_{DW}$ the fractional vortices in addition to their logarithmic interaction are bound also by domain walls (with a finite free energy per unit length) which connect them with each other.

Therefore the two available possibilities are $T_{DW} < T_{FV}$ and a single phase transition, whereas the scenario with $T_{DW} > T_{FV}$ is impossible. Analogous conclusions have been earlier achieved in relation with hypothetical unbinding of fractional vortices in planar antiferromagnet with triangular lattice.¹⁰ It is hardly surprising that the same conclusions are valid for the system, the ground state of which is practically identical to that of the antiferromagnetic XY model with triangular lattice, the only difference being that one quarter of sites is absent.

The proliferation of the low energy domain walls [of the type shown in Fig. 3(b)] leads to intermixing of six different states [which can be obtained from the state shown in Fig. 2(a) by arbitrary permutation of A, B, and C] and therefore should not be expected to be of the Ising type. Note that the domain walls are possible only between the states with the different signs of staggered chirality. The six-state model with analogous statistics of domain walls can be defined¹⁰ by the partition function

$$Z = \left(\prod_{\mathbf{R}} \sum_{t_{\mathbf{R}}=1}^6 \right) \prod_{\mathbf{NN}} W(t_{\mathbf{R}} - t_{\mathbf{R}'}), \quad (22)$$

where

$$W(t) = \begin{cases} 1 & \text{for } t=0 \pmod{6} \\ w & \text{for } t=1,3,5 \pmod{6} \\ 0 & \text{for } t=2,4 \pmod{6}. \end{cases} \quad (23)$$

The last line of Eq. (23) implies that the domain wall between the states with the same parity of $t_{\mathbf{R}}$ is impossible.

Application of the duality transformation³⁵ to the partition function (22) transforms it into analogous partition function with $W(t)$ replaced by

$$\tilde{W}(t) = \begin{cases} 1+3w & \text{for } t=0 \pmod{6} \\ 1 & \text{for } t=1,2,4,5 \pmod{6} \\ 1-3w & \text{for } t=3 \pmod{6}. \end{cases} \quad (24)$$

The symmetry of $\tilde{W}(t)$ corresponds to the so-called cubic model, the phase transition in the six-state version of which for $\tilde{W}(1) > \tilde{W}(3)$ is known to be of the first order.³⁶ The phase transition at T_{DW} in our system (at least when it happens at $T_{\text{DW}} < T_{\text{FV}}$) therefore also can be expected to be of the first order.

Comparison of the estimate Eq. (21) with Eq. (11) shows that the fulfillment of the relation $T_{\text{DW}} < T_{\text{FV}}$ requires $0 < -J_2 < J_{\text{max}}$, where J_{max} can be estimated to be of the order of $10^{-3}J_1$. For $-J_2 > J_{\text{max}}$ there should be only one phase transition in the system, at which the proliferation of domain walls is accompanied by the unbinding of all types of vortices. A detailed description of how it happens still remains to be constructed, but when the dissociation of pairs of fractional vortices is forced by the disappearance of their linear interaction (mediated by the domain walls which connect them) at temperatures, for which their logarithmic interaction is already too weak, one can expect the value of the helicity modulus at T_c to be nonuniversal:

$$\frac{2}{\pi} < \frac{\Gamma(T_c)}{T_c} < \frac{18}{\pi}. \quad (25)$$

Note that the estimate for J_{max} has been found by taking the estimate Eq. (21) on its face value, that is without the unknown numerical coefficient, and therefore should be considered with great caution.

V. THE CASE OF THE ANTIFERROMAGNETIC NNN INTERACTION

For the antiferromagnetic sign ($J_2 > 0$) of the NNN interaction the minimum of the Hamiltonian Eq. (2) is achieved in one of the states with the ferromagnetic ordering of chiralities [Fig. 2(b)]. Such state also allows for construction of a domain wall, the energy of which (per elementary link) E_{DW}^+ is proportional to the strength of second neighbor coupling: $E_{\text{DW}}^+ \approx 3J_2$, see Fig. 7(a). However, comparison of Fig. 7(a) with Fig. 7(b) shows that (in contrast to the case considered in Sec. IV) for $J_2 > 0$ the form of the state on the other side of the wall is uniquely defined by the orientation of the wall and is different for different orientations of the wall. The discrepancy in φ that appears when crossing domain walls of different orientations should be taken care of

by the fractional vortices which have to appear on *all* corners of domain walls (the same happens in the fully-frustrated XY model with square lattice¹²). This makes impossible the construction of a closed domain wall the energy of which is determined entirely by J_2 and does not depend on J_1 .

For $J_2 \ll J_1$ a typical thermally excited defect (leading to the change of the sign of chirality) has the form of a long strip formed by two low energy domain walls [Fig. 7(c)]. Like in Fig. 6 the letter X designates the sites with $\varphi \approx (\varphi_A + \varphi_B)/2$. In the vicinity of these sites the values of other variables φ_i slightly deviate from that shown in the figure. Analogous stripe defects are dominant at low temperatures in the frustrated XY-model with triangular lattice and $f = 1/4$ or $f = 1/3$.³⁷

The energy of such defect is given by $2E_0 + 2E_{\text{DW}}^+L$, where $E_0 = c_0J_1$ ($c_0 \approx 0.55$) is the energy of its termination point and L its length. For $J_2 \ll T \ll J_1$ the average length $\langle L \rangle$ of such defects is given by the ratio $T/(2E_{\text{DW}}^+) \gg 1$, whereas

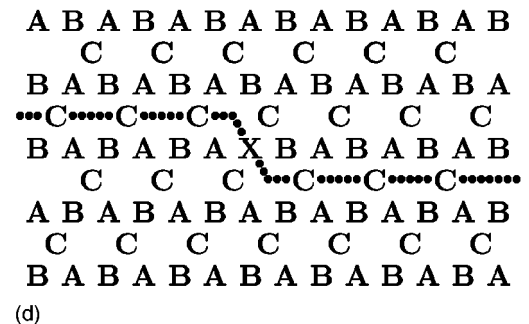
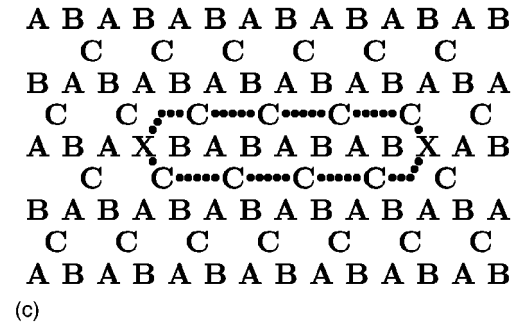
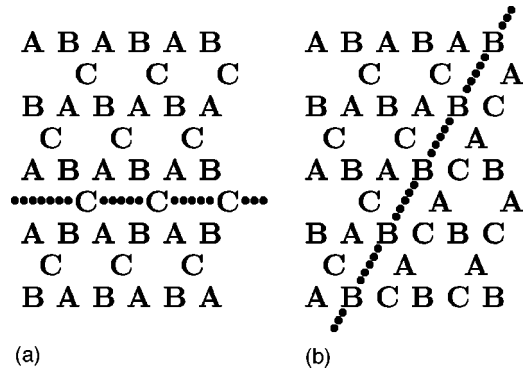


FIG. 7. (a) and (b) two examples of a domain wall separating two $\mathbf{q}=0$ states; (c) a typical finite size defect on the background of $\mathbf{q}=0$ state; (d) a kink on a domain wall.

their concentration c is proportional to $\langle L \rangle \exp(-2E_0/T)$. The relation $c\langle L \rangle^2 \sim 1$ defines the temperature

$$T_* \approx \frac{2}{3} \frac{E_0}{\ln(T_*/E_{\text{DW}}^+)} \quad (26)$$

above which such defects no longer can be considered as independent. The same temperature can serve as the (lower bound) estimate for the temperature T_{DW}^+ of the phase transition associated with proliferation of the domain walls and leading to destruction of the long-range order in chirality. For $J_2/J_1 \rightarrow 0$

$$T_{\text{DW}}^+ \sim T_* \propto J_1 / \ln(J_1/J_2). \quad (27)$$

Analogous estimate can be obtained by comparison of the domain wall energy E_{DW}^+ with its entropy $S_{\text{DW}}^+ \approx 2 \exp(-E_K/T)$ due to possibility of formation of kinks [Fig. 7(d)]. The energy of a kink E_K is very close to E_0 . The requirement $F_{\text{DW}}^+ \equiv E_{\text{DW}}^+ - TS_{\text{DW}}^+ = 0$ ³² gives

$$T_{\text{DW}}^+ \sim E_K / \ln(2T_{\text{DW}}^+/E_{\text{DW}}^+) \quad (28)$$

which is again the estimate from below.

Like in the previous case (of the antiferromagnetic ordering of chiralities) the proliferation of domain walls can take place as the independent phase transition only at temperatures lower than T_{FV} . Comparison of Eq. (28) with Eq. (11) shows that the fulfillment of relation $T_{\text{DW}}^+ < T_{\text{FV}}$ requires $J_2 < J_{\text{max}}^+$, where J_{max}^+ can be estimated as $(10^{-4} \div 10^{-5})J_1$. Also like in the previous case, the proliferation of domain walls is related with intermixing of six different states and therefore can hardly be expected to demonstrate the Ising type behavior.

VI. SPIN WAVE FLUCTUATIONS

Another mechanism for removal of accidental degeneracy (which is traditionally referred to as ‘‘ordering due to disorder’’³⁸) is related with the free energy of continuous fluctuations (spin waves).³⁹ Expansion of the Hamiltonian (1) up to the second order in deviations $\psi_i \equiv \varphi_i - \varphi_i^{(0)}$ of the variables φ_i from their values $\varphi_i^{(0)}$ in some ground state gives the same answer

$$H^{(2)} = \frac{J_1}{4} \sum_{\text{NN}} [-1 + (\psi_i - \psi_j)^2] \quad (29)$$

for all possible ground states, which means that the difference in the free energy between them can appear only in the second order in temperature.¹ That is believed to be not sufficient for stabilization of a true long-range order related with chiralities. This conclusion does not take into account the peculiarities of the statistical mechanics of the considered system and has to be corrected.

With the help of the numerical calculation (see the Appendix) we have found that the lowest order contribution to the effective interaction of chiralities of neighboring triangular plaquettes is of the antiferromagnetic sign (that is favors $\sqrt{3} \times \sqrt{3}$ state) and corresponds to

$$E_{\text{DW}}^{(0)} = \gamma \frac{T^2}{J_1} \quad (30)$$

where $\gamma \approx 2 \times 10^{-3}$. Thermal⁴⁰ and quantum⁴¹ anharmonic fluctuations in Heisenberg *kagomé* antiferromagnet are also known to favor (at least locally) a planar state with $\sqrt{3} \times \sqrt{3}$ structure. The same can be said about the fluctuations of the order parameter amplitude in superconducting wire networks.⁴²

Although $E_{\text{DW}}^{(0)}$ defined by Eq. (30) is always much smaller than the temperature and in the case of (for example) Ising model would be insufficient for appearance of the long-range order, in the considered system the situation is qualitatively different. Substitution of Eq. (30) into Eq. (21) gives a finite value of T_{DW} induced by spin wave fluctuations:

$$T_{\text{DW}}^{(0)} \sim \gamma^{3/2} J_1 \quad (31)$$

which means that for $\gamma \sim 1$ the long-range order in staggered chirality would survive even up to $T \sim J_1$. However, substitution of the numerically calculated value of γ cited above produces an extremely low estimate: $T_{\text{DW}}^{(0)} \sim 10^{-4} J_1$.

Note that the ordering in staggered chirality is noticeable only at length-scales larger than the correlation radius ξ . Substitution of Eq. (30) into Eq. (20) shows that for $T \ll T_{\text{DW}}^{(0)}$ the behavior of $\xi(T)$ is given by $\ln \xi \propto (J_1/\gamma T)^{\bar{\nu}}$. That means that at $T \rightarrow 0$ there takes place a continuous re-entrant phase transition into the phase without true long-range order in staggered chirality.

VII. CONCLUSION

This work has been devoted to investigation of the phase transitions in the antiferromagnetic *XY* model on a *kagomé* lattice with the special emphasis on accurate consideration of mutual influence between different classes of topological excitations (fractional vortices and domain walls). In particular, we have shown that in the model with only NN interaction the additional interaction of fractional vortices related with the entropic contribution from zero-energy domain walls at finite temperatures becomes short-ranged. Therefore it cannot interfere with the BKT dissociation of fractional vortex pairs proposed in Refs. 1 and 13.

For the case of a finite NNN coupling (leading to removal of the accidental degeneracy) we have demonstrated that the phase transition related with proliferation of the domain walls can happen as a separate phase transition below T_{FV} only for very weak NNN interaction, and have found how the temperature of this transition depends on J_1 and J_2 . These dependencies are essentially different for different signs of the NNN coupling. The same results are also applicable for other mechanisms of removal of the accidental degeneracy, which lead to a finite E_{DW} . Note that our analysis has been restricted to the case $|J_2| \ll J_1$, so we have not yet mentioned the possibility of the domain wall proliferation happening above the temperature of the ordinary BKT transition, associated with appearance of free integer vortices (like it happens in the case of triangular lattice^{10,43,44}).

Our conclusions are compatible with the results of the

numerical simulations of Geht and Bondarenko,⁵ who have found (for not too weak NNN interaction, $|J_2| \geq 0.1J_1$) that the disordering of all degrees of freedom in the antiferromagnetic XY model with *kagomé* lattice takes place at the same temperature, the singularities of the thermodynamic quantities being of the Ising type. Recently it has been shown⁴⁴ (for the case of triangular lattice) that when the domain wall proliferation happens as a continuous phase transition [at $T/\Gamma(T) > 2T_{FV}/\Gamma(T_{FV})$], the dissociation of pairs of integer vortices has to take place at $T < T_{DW}$. Since the same arguments are also applicable for a *kagomé* antiferromagnet with $J_2 < 0$, it may be of interest to check the results of Ref. 5 with better accuracy.

The long-range order in staggered chirality is favored also by the spin-wave fluctuations. Our analysis suggests that the antiferromagnetic XY model with *kagomé* lattice and only NN interaction presents a unique example of a model without free parameter in which one of the phase transitions can be expected to happen at dimensionless temperature of the order of 10^{-4} . Therefore one can conclude that the numerical simulations of Rzechowski²³ have demonstrated no evidence for selection of a single ground state down to $T/J_1 \approx 10^{-3}$ not because $E_{DW} \propto T^2/J_1$ is not sufficient for that, but simply because the temperature was not low enough. Comparison with Eq. (27) shows that if the effective interaction of chiralities, induced by the free energy of spin waves, would be of the opposite sign, the long-range order in chirality would persist up to much higher temperatures.

All these features are summarized in Fig. 8, which very schematically (not in scale) shows the structure of the phase diagram of the considered model. The phases with ferromagnetic and antiferromagnetic ordering of chiralities are denoted F and AF, respectively. The phase without long-range order in terms of chiralities, but with quasi-long-range order in terms of $\exp(i3\varphi)$ is denoted S, and the completely disor-

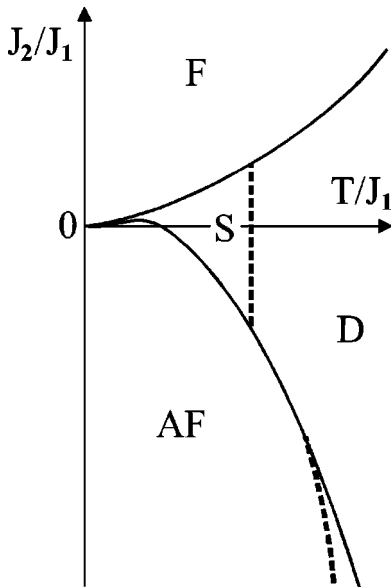


FIG. 8. Schematic phase diagram of the antiferromagnetic XY model with a *kagomé* lattice which follows from the results of this work.

dered phase D. Dashed lines show the phase transitions of the BKT type related with unbinding of pairs of fractional (the border between S and D) or integer (in the lower part of phase diagram) vortices. Quite remarkably, for extremely small positive J_2 the system has to experience with increase in temperature four phase transitions following the path $F - S - AF - S - D$.

Experimentally the phase transitions discussed in this work can be observed in superconducting wire networks or Josephson junction arrays in the external magnetic field providing one-half of the superconducting flux quantum $\phi_0 = hc/2e$ per each triangular plaquette of a *kagomé* lattice. In such systems the removal of the accidental degeneracy is related with the magnetic interaction of the currents and a finite width of the wires.⁴² The former of these mechanisms favors the ferromagnetic ordering of chiralities, whereas for the latter the effect depends on the width of the wires.

Recent experimental investigation of the aluminum wire network with *kagomé* structure¹⁶ has demonstrated for $\phi = \phi_0/2$ the presence on the current-voltage curve of the regions corresponding to different mechanisms of dissipation, one of which (with an algebraic behavior) can be associated with unbinding of vortex pairs and the other with spreading of domains with inverted chiralities.⁴⁵ The authors of Ref. 16 have interpreted this as an evidence for the presence of two phase transitions, although appearance of a new phase transition should be associated with a change of behavior at small rather than at finite currents. Note that the whole region of the existence of the phase S is very narrow ($-10^{-3} \leq J_2/J_1 \leq 10^{-4}$), so the observation of this phase in the experimental situation requires an almost exact cancellation of contributions to J_2 related with different mechanisms (see also Ref. 42).

ACKNOWLEDGMENTS

This work has been supported in part by the Program “Statistical Physics” of the Russian Ministry of Science, by the Program “Scientific Schools of the Russian Federation” (Grant No. 00-15-96747), by the Swiss National Science Foundation, and by the Netherlands Organization for Scientific Research (NWO) in the framework of Russian-Dutch Cooperation Program. The author is grateful to A. V. Kashuba for useful discussion and to I. V. Andronov for assistance in preparation of the figures.

APPENDIX

The lowest order contribution to the interaction of chiralities of neighboring triangular plaquettes induced by the spin wave free energy appears when the partition function of the Hamiltonian (1) is expanded up to the second order in

$$H^{(3)} = \frac{J_1}{6} \sum_{\text{NN}} [\sin(\varphi_i - \varphi_j)] (\psi_i - \psi_j)^3, \quad (\text{A1})$$

and then is averaged with the help of $H^{(2)}$. The fourth-order term is the same for all the ground states and therefore of no importance.

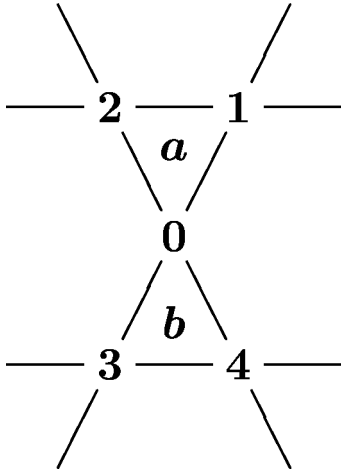


FIG. 9. The numbering of sites used in the expressions for $H_a^{(3)}$ and $H_b^{(3)}$.

The parameter J_p describing the effective interaction of chiralities of neighboring triangular plaquettes (a and b):

$$E(\sigma_a, \sigma_b) = J_p \sigma_a \sigma_b \quad (\text{A2})$$

can be then found by calculating the average of

$$V = -\frac{H_a^{(3)} H_b^{(3)}}{T}, \quad (\text{A3})$$

where

$$H_a^{(3)} = \frac{\sin \frac{2\pi}{3}}{6} J_1 [(\psi_1 - \psi_0)^3 + (\psi_2 - \psi_1)^3 + (\psi_0 - \psi_2)^3] \quad (\text{A4})$$

and expression for $H_b^{(3)}$ can be obtained by replacing in Eq. (A4) ψ_1 by ψ_3 and ψ_2 by ψ_4 . The indices from 0 to 4 are used here to denote the five sites belonging to a pair of neighboring triangular plaquettes as shown in Fig. 9.

With the help of the Wick's theorem and symmetry arguments the average of V can be reduced to the form

$$\langle V \rangle = \frac{3J_1^2}{4T} (G_4^3 - 2G_4^2 G_3 + 2G_4 G_3^2 - G_3^3), \quad (\text{A5})$$

where

$$G_3 = g_{01} - \frac{g_{13}}{2}, \quad G_4 = g_{01} - \frac{g_{14}}{2} \quad (\text{A6})$$

and

$$g_{ij} \equiv \langle (\varphi_i - \varphi_j)^2 \rangle \quad (\text{A7})$$

describes the amplitude of fluctuations of $\varphi_i - \varphi_j$ calculated with the help of the harmonic Hamiltonian (29).

The value of g_{ij} for the nearest neighbors (g_{01}) can be calculated exactly:

$$g_{01} = \frac{T}{J_1}, \quad (\text{A8})$$

whereas numerical calculation of the integrals over Brillouin zone defining g_{13} and g_{14} gives

$$g_{13} = \left(\frac{3}{2} + \delta\right) \frac{T}{J_1}, \quad g_{14} = \left(\frac{3}{2} - \delta\right) \frac{T}{J_1}, \quad (\text{A9})$$

where $\delta \approx 0.0213$.

Substitution of Eqs. (A8)–(A9) into Eqs. (A5)–(A6) then gives

$$J_p = \frac{\gamma T^2}{2J_1}, \quad (\text{A10})$$

where

$$\gamma = \frac{3}{32} \delta (1 + 12\delta^2) \approx 2.01 \cdot 10^{-3} \quad (\text{A11})$$

which leads to Eq. (30).

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