Journal of Statistical Physics, Vol. 43, Nos. 1/2, 1986

Phase Transitions in Two-Dimensional Uniformly Frustrated *XY* Models. I. Antiferromagnetic Model on a Triangular Lattice

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Received August 30, 1985

A most popular model in the family of two-dimensional uniformly-frustrated *XY* models is the antiferromagnetic model on a triangular lattice [AF *XY*(t) model]. Its ground state is both continuously and twofold discretely degenerated. Different phase transitions possible in such systems are investigated. Relevant topological excitations are analyzed and a new class of such (vortices with a fractional number of circulation quanta) is discovered. Their role in determining the properties of the system proves itself essential. The characteristics of phase transitions related to breaking of discrete and continuous symmetries change. The phase diagram of the "generalized" AF *XY*(t) model is constructed. The results obtained are rederived in the representation of the Coulomb gas with half-integer charges, equivalent to the AF *XY*(t) model with the Berezinskii-Villain interaction.

KEY WORDS: Two-dimensional systems; phase transitions, frustrated *XY* models; antiferromagnetic *XY* model; topological excitations; fractional vortices; Coulomb gas; Josephson junctions.

1. INTRODUCTION

It is well-known[1-4] that no rigorous long-range order can exist in two-dimensional systems characterized by a continuous group of symmetry. Nevertheless, as has been shown by Berezinskii,[5] in the systems with an Abelian group of symmetry the so-called quasi-long-range order (an algebraic decay of correlation functions) persists at low temperatures. The nature of the phase transition to a high-temperature phase with an exponential decay of correlation functions has been elucidated by

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0022-4715/86/0400-0001$05.00/0

Berezinskii,[6–7] Kosterlitz and Thouless[8] and Kosterlitz.[9] This transition is related to dissociation of pairs of topological excitations (vortices); at low temperatures all the vortices are bound in pairs, but at some temperature, estimated by Kosterlitz and Thouless,[8] a plasma of free vortices is formed.

A rather popular application of this theory is the description of lattice systems of two-component (planar) spins with ferromagnetic interaction (XY model)

$$H = J \sum_{(\mathbf{r}\mathbf{r}')} \mathbf{s}_\mathbf{r} \mathbf{s}_{\mathbf{r}'} \tag{1.1}$$

where $J < 0$ denotes the exchange coupling, and $\mathbf{s}_\mathbf{r} = (\cos \varphi_\mathbf{r}, \sin \varphi_\mathbf{r})$ is a two-component unit spin vector. Summation in (1.1) is performed over the pairs of nearest neighbors on a regular two-dimensional lattice. Hamiltonian (1.1) can be expressed in terms of the variables $\varphi_\mathbf{r}$ in the form

$$H = J \sum_{(\mathbf{r}\mathbf{r}')} \cos(\varphi_\mathbf{r} - \varphi_{\mathbf{r}'}) \tag{1.2}$$

The particular structure of the lattice becomes important for the case of an antiferromagnetic (AF) interaction ($J > 0$). The partition function of the AF model on a square lattice can be reduced to that of a ferromagnetic model by the substitution $\mathbf{s} \to -\mathbf{s}$ for one of the two sublattices, but this does not hold for the case of a triangular lattice. The AF XY model on a triangular lattice (AF XY(t) model) is a frustrated one; for $J > 0$ one cannot minimize all the terms in the Hamiltonian (1.1) simultaneously. The ground state of this system is well known: it contains three equivalent sublattices, their spins being rotated by the angle 120° in respect to each other

$$\varphi_2 = \varphi_1 + 120°, \qquad \varphi_3 = \varphi_2 + 120° \tag{1.3a}$$

or

$$\varphi_2 = \varphi_1 - 120°, \qquad \varphi_3 = \varphi_2 - 120° \tag{1.3b}$$

The ground state is twofold discretely degenerated, in addition to the continuous degeneration caused by the possibility of homogeneous spin rotation. Consequently, the symmetry group of AF XY(t) magnet is $U(1) \times Z_2$, and the order parameter degeneracy space can be presented as two disconnected circumferences.

Notwithstanding the recent active investigations,[10–14] the question of the nature and succession of phase transitions in the system under investigation has still remained to be elucidated. In this paper we have analyzed the problem by studying the properties of relevant topological excitations in conventional and Coulomb gas representations.

The AF $XY(\mathrm{t})$ model investigated here belongs to a wide class of uniformly frustrated XY models, whose Hamiltonian has the form:

$$H = -J \sum_{(\mathbf{rr}')} \cos(\varphi_{\mathbf{r}} - \varphi_{\mathbf{r}'} - \psi_{\mathbf{rr}'}) \tag{1.4}$$

with the constraints:

$$\sum_{\Gamma_l} \psi_{\mathbf{rr}'} = 2\pi f, \qquad l = 1, 2, ..., N \tag{1.5}$$

imposed on fixed constants $\psi_{\mathbf{rr}'}(\psi_{\mathbf{r}'\mathbf{r}} \equiv -\psi_{\mathbf{rr}'})$. Summation in (1.5) is performed along the perimeter of each elementary plaquette Γ_l, their number being N. Since the interaction entering into the Hamiltonian (1.4) is a periodic and even function, it is sufficient to assume $f \in [0, \frac{1}{2}]$. For f lying outside the segment $[0, \frac{1}{2}]$ the problem can be reduced to analyzing $f \in [0, \frac{1}{2}]$ by redefinition of the phase $\varphi_{\mathbf{r}}$. The AF $XY(\mathrm{t})$ model (all $\psi_{\mathbf{rr}'} = \pi$) corresponds to $f = \frac{1}{2}$.

As has been mentioned above, the ground state of the AF $XY(\mathrm{t})$ model can be of two kinds (see Eqs. (1.3a) and (1.3b)). In both cases the angle φ rotates by 360°, when the plaquette is passed around, i.e., each triangle is characterized by its own helicity (vorticity) $h = \pm 1$. In the ground state the helicities with opposite signs form an alternating regular structure.

The above definition of helicity means that its value is calculated with respect to the ferromagnetic state of the plaquette. Such a definition has been use in all the previous papers. It turns out to be inconvenient for considering topological excitations of the domain wall-type in the AF $XY(\mathrm{t})$ model and in more general uniformly frustrated models.

It seems appropriate to calculate helicity in the following manner

$$h = \frac{1}{2\pi} \sum_{\Gamma_l} \{\varphi_{\mathbf{r}} - \varphi_{\mathbf{r}'} - \psi_{\mathbf{rr}'}\} \tag{1.6}$$

where $\{\cdots\}$ denotes the value reduced to the interval $(-\pi, \pi)$. In the case of the AF $XY(\mathrm{t})$ model this procedure corresponds to calculation of helicity on the background of an ideal AF state, which cannot be achieved for a frustrated model. In this case $h = \pm\frac{1}{2}$, and in the general case of the model (1.4)–(1.5) in the ground state we get $h = 1 - f, -f$.

The properties of a two-dimensional AF $XY(\mathrm{t})$ magnet are not of academic interest only. In particular, such properties should be displayed by a dense monolayer of O_2 on a graphite substrate[15] and also by layers of Eu intercalated into graphite.[16]

For the last few years it has become possible to observe experimentally the phase transitions typical for uniformly-frustrated XY models in regular arrays of Josephson junctions.[17–20] These devices contain a macroscopically great number of superconducting elements, which form a regular lattice and are weakly coupled with each other. The resistive state in those devices placed in an external transverse magnetic field displays very peculiar low-temperature behavior when varying the magnitude of the flux ϕ per an elementary cell. The theoretical description of such systems (see, for instance, Refs. (21–23)) can be realized by means of the frustrated XY models with the Hamiltonian given by (1.4)–(1.5), where

$$\psi_{\mathbf{rr}'} = \frac{2\pi}{\phi_0} \int_{\mathbf{r}'}^{\mathbf{r}} \mathbf{A}\, d\mathbf{l} \tag{1.7}$$

and $\phi_0 = \pi\hbar c/e$ is the flux quantum.

The present paper is organized as follows. Section 2 is devoted to elucidation of the nature of topological excitations in the AF XY(t) model: integer vortices, domain walls, fractional vortices. In the problem considered, two energy parameters can be introduced—the energy of the domain wall per unit length and the prelogarithmic factor in the vortex–vortex interaction. The ratio of these parameters turns out to determine what kinds of phase transition are possible. The phase diagram is constructed. In the following section the same AF XY(t) model is discussed in terms of the Coulomb gas representation. A number of other examples of uniformly frustrated XY models and phase transitions possible in them are analyzed in Part II, which is published as a separate paper.[24]

In this paper we study phase transitions in an AF XY(t) magnet for zero magnetic field only. An analysis of the phase diagram of the AF XY(t) magnet in an external magnetic field presents another interesting problem[11–13] which is consisdered elewhere.[25]

2. TOPOLOGICAL EXCITATIONS AND PHASE TRANSITIONS IN THE AF *XY*(t) MODEL

The partition function of the model with a continuously degenerated symmetry has a form of a functional integral. The evaluation of the partition function by means of the saddle-point method requires that aside from the ground state, the states corresponding to the Hamiltonian local minima and also the fluctuations in their vicinities should be considered. In the model under consideration the number of local minima of the

Hamiltonian includes such topologically stable excitations as vortices and domain walls.

The vortex in an AF XY(t) magnet can be thought of as vortex in a ferromagnet in which spins are rotated by the angles φ_n; the same for each sublattice. The values of these angles φ_n are equal to those in the ground state of an AF magnet. At low temperatures the vortices are bound into small pairs.

The domain walls (Fig. 1) are also relevant topological excitations. The states of both sides of the wall belong to two above-mentioned dif-

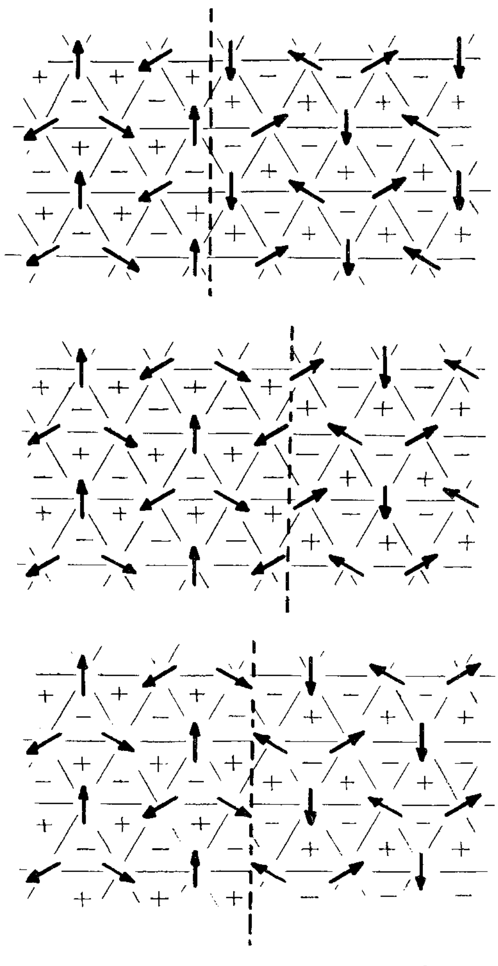

Fig. 1. Domain walls in an AF XY(t) magnet. The states to the left from the walls are the same. The states to the right from the walls depend on the position of the wall and can be transformed one into another by rotation through 120°. The signs + and − denote the signs of helicities equal to $\pm\frac{1}{2}$, calculated by Eq. (1.6).

ferent circumferences of the order parameter degeneracy space. If on one side of the wall the spin distribution can be described by formulas (1.3a) (far from the wall), on the other side it should be described by formulas (1.3b). A more accurate treatment of the domain wall, as a Hamiltonian extremum, shows that the states on both sides from the wall, given by formulas (1.3a) and (1.3b), respectively, should satisfy the condition

$$\Delta\varphi_1 \equiv \varphi_1^a - \varphi_1^b = 60°, 180°, 300° \tag{2.1}$$

The particular value in the right-hand side of (2.1) is dependent on the position of the wall. For the given value of $\Delta\varphi_1$ the values of $\Delta\varphi_2$ and $\Delta\varphi_3$ are determined unambiguously by (1.3). These three possibilities are illustrated in Fig. 1.

As has been mentioned above the order parameter degeneracy space can be presented as two circumferences. Each point of one of them is connected with three points on another circumference by equivalent extremal paths (domain walls). Consequently, all the points of degeneracy spaces can be grouped as families, consisting of six points (three on each circumference) mutually connected by extremal paths. One of these families is schematically shown in Fig. 2.

There are local minima of Hamiltonian (1.1) of more complex structures than those considered so far. They can be treated as a superposition of a domain wall with a kink and of a vortex with a noninteger number of circulation quanta, the vortex being localized on the kink. Such a vortex arises as compensation of the spin orientation discrepancy on both sides of the kink. Figure 3 presents schematically a domain wall with a kink and the angles of spin rotation on both sides of the wall. Since while passing around the kink (for instance, along contour Γ in Fig. 3) the angles at the

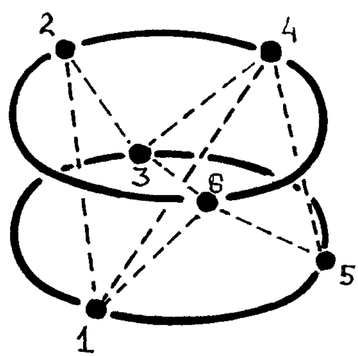

Fig. 2. Order parameter degeneracy space of the AF $XY(t)$ magnet. One of the families consisting of six points connected through extremal paths is indicated.

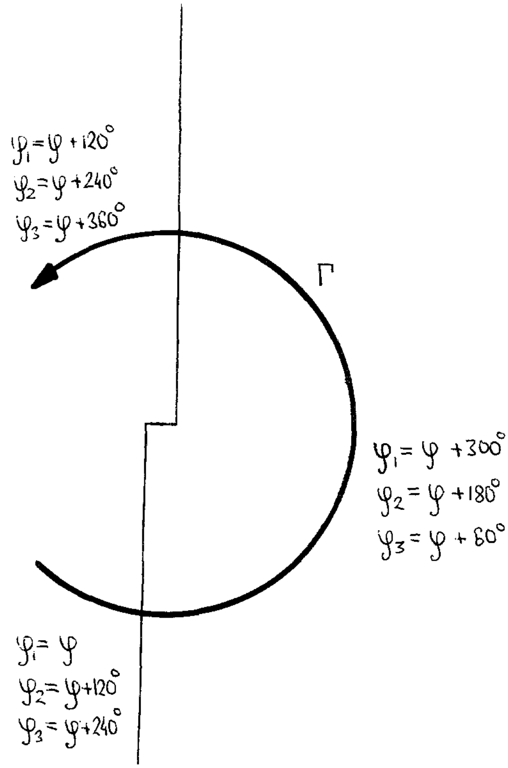

Fig. 3. A domain wall with the kink upon which a fractional vortex should be localized.

points of intersection of the domain wall and the contour undergo jumps of different values, there arises inconsistency of 120°, which should be compensated by a fractional vortex. Fractional vortices can be localized also at the wall bends and at the points of their intersection.

Let us now discuss possible phase transitions related to the indicated topological excitations. It is a popular idea (see, for instance, ref, 10) that since AF XY(t) model's symmetry group is $U(1)\times Z_2$, two different phase transitions are possible: the Ising transition and Berezinskii–Kosterlitz–Thouless dissociation of conventional (integer) vortices, so the problem is reduced to the elucidation of their successsion. The situation turns out to be not so simple.

Indeed, one of the possibilities pointed out by Dotsenko and Uimin[13] as the only appropriate one assumes that with increasing temperature the Berezinskii–Kosterlitz–Thouless transition[5–9] (BKT transition) is the first to occur. It is related with the dissociation of pairs of ordinary (interger) vortices. On a dual lattice this transition manifests itself in the formation of a "neutral plasma" of positive and negative vortices on the background of ordered configuration corresponding to one of the circumferences in Fig. 2. In this case the order parameter degeneracy space reduces to Z_2. With further increasing temperature the Ising type phase transition takes place, caused by the vanishing of the domain wall free energy.

Another situation, when the "domain wall" transition is the first to occur, has been mentioned by Lee *et al.*[12] It is noteworthy that a change in the sequence of phase transitions causes change of their types as well. In this case, under the first transition each six-point family of the type shown in Fig. 2 converges into a single point. That leads to reducing the order parameter degeneracy space to a single circumference of $2\pi/3$ in length. The symmetry of the system becomes higher and not only group Z_2 but also group Z_3, which is a discrete subgroup of $U(1)$, are restored. Partial restoration of a spontaneously broken continuous symmetry has been shown to be possible[26] on an example of a particular modification of the ferromagnetic XY model, applied for description of superfluid ^{3}He thin films.

When domain walls with infinite length appear, and more exactly, when the concentration of such walls is finite, the fractional vortices becomes relevant topological excitations instead of integer vortices. This is in accordance with order parameter degeneracy space being reduced in the above-mentioned manner. With further increasing temperature a BKT transition in the system of fractional vortices with circulation $\pm 2\pi/3$ should take place.

There exists a third possibility. The free energy of domain walls vanishes at a certain temperature, when the interaction of integer vortices is still strong enough for them to be bound in pairs (in the absence of fractional vortices), whereas the interaction of fractional vortices is insufficient for formation of bound states. In this case all the group of symmetry $U(1) \times Z_2$ is restored simultaneously, i.e., there appear at once both the infinitely long domain walls and free vortices (fractional and integer). This should take place by means either of the first order phase transition, or of a novel critical behavior, as was supposed by Lee *et al.*[12]

Let us consider in detail the phase transition resulting in formation of infinite domain walls, taking place at those temperatures when fractional vortices are bound in pairs. Though these pairs, and the spin waves as well, let the order parameter vary continuously, a discrete variable $\sigma(\mathbf{r})$, whose value changes only when crossing the wall, can be introduced on the background of this continuous variation. The domain wall separates the states belonging to different circumferences (Fig. 2). The domain wall transition can be described qualitatively by the lattice model with a short-range interaction, in which the discrete variables $\sigma(\mathbf{r})$ acquire six different values (for instance, $\sigma(\mathbf{r}) = 1, 2, \ldots, 6$). The symmetry of such a model should be $Z_3 \times Z_2$, and not Z_6. The weight function corresponding to the nearest neighbor interaction should have a form

$$\begin{aligned} W(\sigma-\sigma') &= 1 & \sigma-\sigma' &= 0 \pmod 6 \\ &= w & \sigma-\sigma' &= 1 \pmod 6 \\ &= 0 & \sigma-\sigma' &= 2 \pmod 6 \\ &= w & \sigma-\sigma' &= 3 \pmod 6 \\ &= 0 & \sigma-\sigma' &= 4 \pmod 6 \\ &= w & \sigma-\sigma &= 5 \pmod 6 \end{aligned} \tag{2.2}$$

where $w = \exp(-J_W/T)$ and J_W is the energy per a unit length of the domain wall. Equation (2.2) means that the domain wall can separate only the states with different parity of the variable.

In case a dual transformation[27] is performed for model (2.2), we obtain a model with an analogous structure of Hamiltonian, but with the weight function

$$\begin{aligned} \tilde{W}(\tau-\tau') &= 1+3w & \tau-\tau' &= 0 \pmod 6 \\ &= 1 & \tau-\tau' &= 1 \pmod 6 \\ &= 1 & \tau-\tau' &= 2 \pmod 6 \\ &= 1-3w & \tau-\tau' &= 3 \pmod 6 \\ &= 1 & \tau-\tau' &= 4 \pmod 6 \\ &= 1 & \tau-\tau' &= 5 \pmod 6 \end{aligned} \tag{2.3}$$

This form of the weight function displays cubic symmetry of the dual order parameter τ. We can interpret τ as a unit vector which is parallel or antiparallel to the three mutually perpendicular coordinate axes. If we assume that a unit weight function corresponds to mutually parallel τ, then the weight function $W_{\uparrow\rightarrow} = 1/(1+3w)$ corresponds to perpendicular τ, and $W_{\uparrow\downarrow} = (1-3w)/(1+3w)$ to antiparallel ones. In a $2n$-state cubic model for $n > 2$ and $W_{\uparrow\rightarrow} > W_{\uparrow\downarrow}$ the phase transition is of the first order.[28] Our case corresponds to $n = 3$. The phase transition point of the $2n$-state Potts model (corresponding to the case $W_{\uparrow\rightarrow} = W_{\uparrow\downarrow}$) also belongs to the same line of the first order phase transitions.[28]

Summarizing the results obtained, we enumerate the available possibilities:

1. BKT transition, and with further increase in temperature the Ising transition.

2. First order transition and then BTK transition in the system of fractional vortices. In this case the value of the helicity modulus of the spin system at the BKT transition point should be equal to $(18/\pi)T$, and not to $(2/\pi)T$, as in the case of a conventional BKT transition.
3. Only one phase transition of the first order or that of a new class of universality.

In the first case no rigidity of a spin system relative to continuous deformation can be observed in the intermediate phase, but "antiferromagnetic" ordering of helicities of opposite signs is retained. In the second case in an intermediate phase the rigidity of the spin system is retained and, though the correlation function $\langle \exp i(\varphi_{\mathbf{r}_1} - \varphi_{\mathbf{r}_2}) \rangle$ decays exponentially at large distances due to existence of infinitely long domain walls (even if $\mathbf{r}_1$ and $\mathbf{r}_2$ are taken to belong to the same sublattice), some other correlation functions, for instance, $\langle \exp i6(\varphi_{\mathbf{r}_1} - \varphi_{\mathbf{r}_2}) \rangle$ are characterized by an algebraic decay. In a high-temperature (disordered) phase all the correlation functions mentioned above decay exponentially.

A qualitative analysis performed above does not make it possible to indicate unambiguously which of these possibilities is realized in model (1.2). The results of numerical simulations[10] reveal the logarithmic behavior of the specific heat and the critical exponents that correspond to the Ising type transition. This indicates unambiguously that the first of the possibilities is realized, so we can conclude that at a lower temperature a conventional BKT transition should take place. This conclusion turns out to be in agreement with the Miyashita and Shiba results.[10]

For realization of other possibilities it is necessary to consider generalization of Hamiltonian (1.2) for the case of some other form of the interaction function, distinct form $J\cos(\varphi_{\mathbf{r}} - \varphi_{\mathbf{r}'})$, or for the case of the interaction of farther neighbors being taken into account. Figure 4 shows schematically a phase diagram of a "generalized" AF XY(t) model. It contains four different phases and is presented in the coordinates T/J_W, T/J_V, where J_W is the domain wall energy, and J_V is the prelogarithmic factor in the vortex–vortex interaction. On line *be* the free energy of a domain wall turns to zero; line *df* corresponds to the dissociation of pairs of fractional vortices. Line *df* terminates on line *be*, since on the other side of *be* the fractional vortices cannot be separated by large distances, being localized on closed domain loops of a limited size. Line *ac* denotes dissociation of ordinary vortex pairs. This line also terminates on line *be*, since on the other side of *be* some other process is responsible for disordering, namely, the dissociation of pairs of fractional vortices. It seems extremely probable that the first order phase transition line *de* of the cubic model will extend further (beyond point *d*) as a first order transition line, since the transition

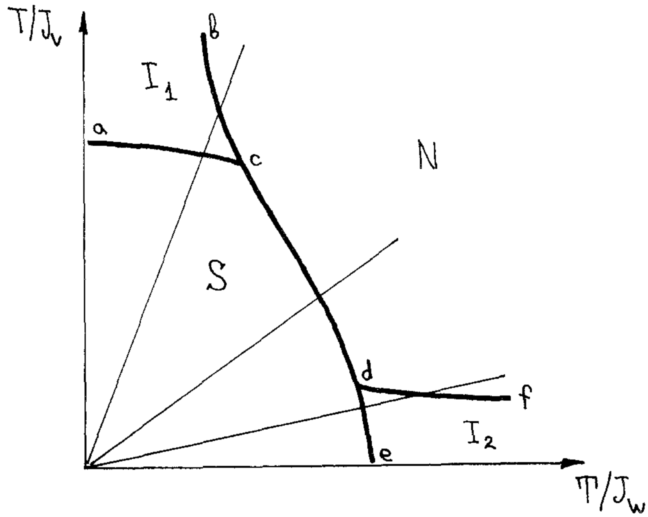

Fig. 4. Phase diagram of the "generalized" AF $XY(\mathrm{t})$ model, N is a disordered phase, S is an ordered phase, I_1 and I_2 are two different intermediate phases.

of fractional vortices to plasma corresponds only to a smoth change in the depth of one of the competing free energy minima.

In Fig. 4 the straight lines passing through the origin of coordinates correspond to thermodynamic paths, i.e., to variation of temperature only, while retaining the form of the interaction ($J_W = \text{const}$, $J_V = \text{const}$). Depending on the slope they intersect one or two lines of phase transitions.

The situation when the domain wall transition precedes the dissociation of fractional vortices is possible due to the fact that a special form of interaction function can be chosen such that the energy of the domain wall vanishes, whereas the system possesses the finite helicity modulus even in the presence of a arbitrary number of domain walls.

3. PHASE TRANSITIONS OF THE AF XY(t) MODEL AND THE COULOMB GAS

It has become a tradition to describe the systems with the order parameter having planar symmetry by the Berezinskii–Villain model (BV model).(7,29) In the case of an AF $XY(\mathrm{t})$ magnet the partition function of the BV model has the form

$$Z = \prod_{\mathbf{r}} \left(\int_0^{2\pi} \frac{d\varphi_{\mathbf{r}}}{2\pi} \right) \prod_{(\mathbf{rr}')} \left(\sum_{p_{\mathbf{rr}'} = -\infty}^{\infty} \right) \exp\left\{ -\frac{J}{2T} \left[\varphi_{\mathbf{r}} - \varphi_{\mathbf{r}'} - 2\pi \left(p_{\mathbf{rr}'} + \frac{1}{2} \right) \right]^2 \right\} \tag{3.1}$$

where $(\mathbf{rr}')$ denotes a pair of neighboring lattice sites, and $p_{\mathbf{rr}'}$ are integers. The BV model admits rigorous transformation to the Coulomb gas.[29,30] As a result, we get

$$Z = Z_0 \sum_{\{m(\mathbf{R})\}} \exp\left[-\frac{1}{2}\sum_{\mathbf{R},\mathbf{R}'} m(\mathbf{R})\, G'(\mathbf{R},\mathbf{R}')\, m(\mathbf{R}')\right] \tag{3.2}$$

where summation is performed over "neutral" vortex configurations

$$\sum_{\mathbf{R}} m(\mathbf{R}) = 0;$$

$m(\mathbf{R})$ acquire all the half-integer values (cf. Ref. (31)) and are defined at the sites of a dual (honeycomb) lattice. $G(\mathbf{R}, \mathbf{R}')$ satisfies a discrete analog of the two-dimensional Poisson equation

$$\Delta_{\mathbf{R}} G(\mathbf{R},\mathbf{R}') = -\frac{4\pi^2 J}{T}\,\delta_{\mathbf{RR}'} \tag{3.3}$$

so at large distances the behavior of $G(\mathbf{R}, \mathbf{R}')$ is logarithmic in $|\mathbf{R}-\mathbf{R}'|$.

The generalization of the BV model for the case of a uniformly frustrated XY model with $f \neq \frac{1}{2}$ and its further transformation to the Coulomb gas representation results in the partition function (3.2) in which $m(\mathbf{R})$ acquire the values $(-f + \text{integer})$.[32]

The ground state of the Coulomb gas with half-integer charges on a honeycomb lattice presents an alternating regular structure of charges $+\frac{1}{2}$ and $-\frac{1}{2}$. This is possible only due to the fact that the honeycomb lattice can be divided into two equivalent sublattices. The ground states is double degenerated ("vacua" a and b). Continuous degeneration is lost in the transformation to the Coulomb gas. Such a regular structure of positive and negative charges can be treated as a peculiar ionic crystal.

Let us consider now the defects which can occur on the background of the ground state. The defects of the first type are excessive integer charges (positive or negative) arising, for instance, if $-\frac{1}{2}$ is replaced by $+\frac{1}{2}$ or by $-\frac{3}{2}$ (Fig. 5). The energy of excissive charges is finite for the case of a neutral pair and depends logarithmically on its spacing. It also contains a finite contribution dependent on the value and sign of the excessive charge and on the sign of the background charge in the point where the excessive charge is situated. That is, the "core" energies of the above-mentioned defects are different. At low temperatures all the excessive charges are bound in pairs.

Another class of excitations consists of domain walls separating the regions of vacua a and b (Fig. 5). The neutral domain wall has finite energy

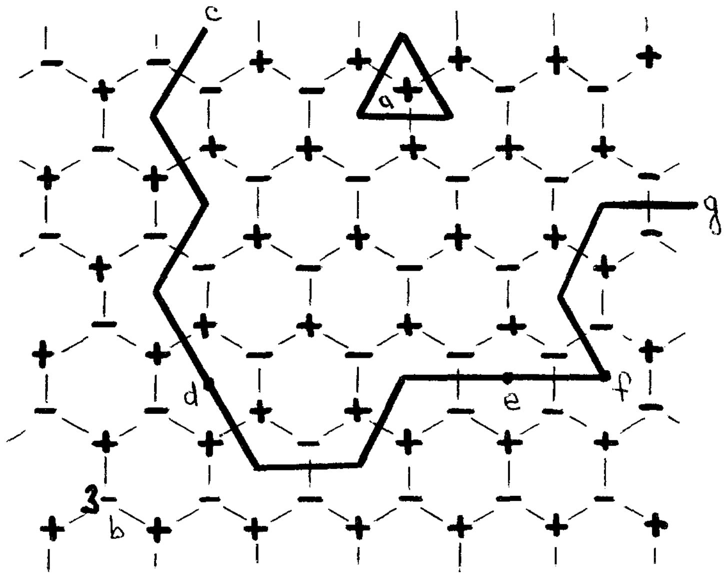

Fig. 5. Coulomb gas of half-integer charges on a honeycomb lattice: defects on the background of the ground state. a and b are excessive charges ($+1$ and -1), cg is the domain wall. Charge $+\frac{1}{3}$ is localized at the point d of the domain wall, and charges $-\frac{1}{3}$ at the point e and f.

per unit length and the energy of its interaction with other domain walls decreases exponentially with distance (see also Section 2 of Ref. 24). At low temperatures only small islands of vacuum b on the background of vacuum a, or vice versa, are present. The domain walls form small closed loops.

With increasing temperature, two phase transitions are possible. They are (1) melting of an ionic crystal, i.e., vanishing of the mean charge of each of two sublattices, and (2) transition of an ionic crystal from a "dielectric" to a "conducting" state, i.e., dissociation of pairs of excessive charges. In the conducting state, the mean square of the charge for the part of the crystal containing an equal number of sites of each sublattice is proportional to the area of this region. In a dielectric state, the fluctuational charge grows with the system size slower. The above transitions are essentially different, and can occur independently.

Let us consider in detail the domain walls in the Coulomb gas representation. The domain wall can be defined as a line passing along the bonds of the initial (triangular) lattice in such a manner that each elementary link of this line divides the two charges of an equal sign (Fig. 5). Provided each two neighboring links of the domain wall form angles of 120°, such a domain wall is neutral. At each site where the neighboring links form angles of 60° or 180° an excessive charge $\pm\frac{1}{3}$ arises (Fig. 5).

The concept of an excessive charge on the background of a regular sign-alternating structure should be of a constructive character, i.e., the charge of the given structural defect should be defined by its interaction with a distant probe charge. The excessive charge can be calculated by the following procedure. Each of the charges of the given state is divided into three equal parts, which are shifted to the centers of three hexagons surrounding the given lattice site. Then all the charges fallen into the center of each of the hexagons are summed up.

In the case of a regular alternation of charges $+\frac{1}{2}$ and $-\frac{1}{2}$ the charges of all the hexagons turn out to be equal to zero. The situation does not change, if there are domain walls, whose neighboring links form the angles of 120°. In the case of other angles each joint has the charge $\pm\frac{1}{3}$. The point of intersection of two domain walls either has no charge at all, or its charge is $\pm\frac{2}{3}$. The point of intersection of three domain walls has the charge ± 1. All the enumerated situations are illustrated in Fig. 6.

In terms of domain walls a simple excessive charge ($+\frac{1}{2}$ instead of $-\frac{1}{2}$) corresponds to an elementary triangular loop, its vertices possessing the charge $+\frac{1}{3}$ each, and the total charge being unity (Fig. 5). For an arbitrarily shaped closed domain wall the charge turns out to be an integer, as can be expected when the signs of some set of half-integer charges (in the inner region of the loop) are changed.

If the phase transition of excessive charges unbinding is the first to take place with an increse in temperature, it is related to the unbinding of integer charges ("independent" or localized on closed domain walls forming

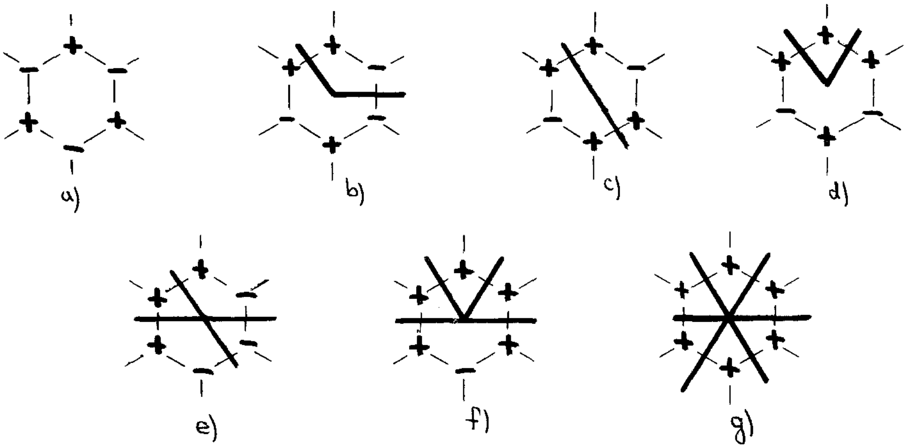

Fig. 6. Excessive charges corresponding to different structures: *a*, regular structure (zero charge); *b*, domain wall (zero charge); *c*, *d*, domain walls (charge $+\frac{1}{3}$); *e*, intersection of two walls (zero charge); *f*, intersection of two walls (charge $+\frac{2}{3}$); *g*, intersection of three walls (charge $+1$).

not too large loops). In the other case if the "melting" of a sign-alternating structure is the first to take place, then a network of infinite domain walls appears which leads to a topological freedom of fractional charges. The second phase transition (if it has not occurred simultaneously with the first one) is now related to dissociation of pairs of charges $\pm\frac{1}{3}$.

Coincidence in classification of defects for an AF XY(t) model and for the Coulomb gas considered proves the reliability of the analysis performed in Section 2, which does not take spin waves into account, and of the phase diagram based on it (Fig. 4). A similar phase diagram should be displayed by the Coulomb gas with the partition function defined by the relation (3.2), when the form of interaction is charged, but its logarithmic character at large distances is retained.

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