Kink Pairs Unbinding on Domain Walls and the Sequence of Phase Transitions in Fully Frustrated *XY* Models

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The unbinding of kink pairs on domain walls in the fully frustrated *XY* model (on square or triangular lattices) is shown to induce the vanishing of phase coupling across the walls. This forces the phase transition, associated with unbinding of vortex pairs, to take place at a lower temperature than the other phase transition, associated with proliferation of the Ising-type domain walls. The results are applicable for a description of superconducting junction arrays and wire networks in a perpendicular magnetic field, as well as of planar antiferromagnets with a triangular lattice.

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A fully frustrated (FF) *XY* model can be defined by the Hamiltonian,

$$H = -J \sum_{(ij)} \cos(\varphi_j - \varphi_i - A_{ij}), \qquad (1)$$

where $J > 0$ is the coupling constant, the fluctuating variables φ_i are defined on the sites i of some regular two-dimensional lattice, and the summation is performed over the pairs of nearest neighbors (ij) on this lattice. The nonfluctuating (quenched) variables $A_{ij} \equiv -A_{ji}$ defined on lattice bonds have to satisfy the constraint $\sum A_{ij} = \pi$ (where the summation is performed over the perimeter of a plaquette) on all plaquettes of the lattice.

For two decades, such models (on various lattices) have been extensively studied in relation to experiments on Josephson junction arrays [1], in which φ_i can be associated with the phase of the superconducting order parameter on the ith superconducting grain, and A_{ij} is related to the vector potential of a perpendicular magnetic field, whose magnitude corresponds to a half-integer number of superconducting flux quanta per lattice plaquette. A planar antiferromagnet with a triangular lattice also can be described by the Hamiltonian (1) (with $A_{ij} \equiv \pm\pi$).

The ground states of the FF *XY* models on square [2] and triangular [3] lattices are characterized by the $U(1) \times Z_2$ degeneracy, which suggests the possibility of two different phase transitions. One of them (the Berezinskii-Kosterlitz-Thouless transition [4–6]) can be associated with unbinding of vortex pairs and the other with proliferation of the Ising-type domain walls.

Teitel and Jayaprakash [7] have proposed that the temperature T_V of the vortex pair dissociation cannot be higher than the temperature T_{DW} of the phase transition associated with domain wall proliferation. The arguments supporting this conjecture have been put forward in Refs. [8–10] and are related to the presence on corners of domain walls of fractional vortices, which are expected to screen the interaction of integer vortices at $T > T_{DW}$.

The application of the Hubbard-Stratanovich transformation [11] to the FF *XY* model on a square lattice allows one to reduce it [12] to the system of two coupled unfrustrated *XY* models, which in the limit of strong coupling becomes equivalent to the so-called *XY*-Ising model:

$$H = -K \sum_{(ij)} (1 + s_i s_j) \cos(\varphi_i - \varphi_j), \qquad (2)$$

where $s_i = \pm 1$ is the auxiliary Ising-type variable. In this model, the coupling of the phase variables φ_i across any domain wall is completely absent. Although this property appears as a direct consequence of taking (without any justification) the strong coupling limit, and such a description fails to take into account the existence of fractional vortices, it has been suggested [13] that the *XY*-Ising model *may* turn out to be a reasonable approximation for investigation of the FF *XY* model.

In the present Letter, we demonstrate that, in the FF *XY* model on square or triangular lattices, the phase transition on a single domain wall, which takes place at $T_K < T_V$ and consists of dissociation of pairs of logarithmically interacting kinks [14], induces for $T > T_K$ the loss of phase coupling across the wall. This indeed makes the behavior of the FF *XY* model analogous to that of the *XY*-Ising model. We also show that the suppression of the phase coupling between different Ising domains leads to $T_V < T_{DW}$, at least when the phase transition associated with domain wall proliferation is a continuous one.

The FF *XY* model on a square (or triangular) lattice being one of the simplest examples of a system with nonperturbative coupling between continuous and discrete degrees of freedom, the results are of interest not only in relation to experimental realizations mentioned above, but in a more general context of two-dimensional statistical mechanics. In particular, we discuss in the conclusion their consequences for the interplay between the roughening and the reconstruction transitions [15,16]. We do not consider here the FF *XY* models on honeycomb [10] and dice [17] lattices, which are characterized by much more developed discrete degeneracies.

In the ground state of the FF *XY* model on a square lattice, the gauge invariant phase differences

$\theta_{ij} = \varphi_j - \varphi_i - A_{ij}$ on all bonds are equal [when reduced to the interval $(-\pi, \pi)$] to $\pm\pi/4$ in such a way that summation of θ_{ij} over the perimeter of each plaquette gives $\pi\sigma$, where $\sigma = \pm 1$ is called chirality. The plaquettes with positive and negative chiralities regularly alternate with each other, forming the checkerboard pattern [2]. The discrete twofold degeneracy of the ground state corresponds to the change of the signs of all chiralities.

A domain wall can be defined as a topological excitation separating two ground states which cannot be transformed into each other by a continuous rotation. Schematically, it can be represented as a line on a lattice, each link of which separates two plaquettes with the same chirality (Fig. 1). A domain wall is characterized by a finite energy per unit length; therefore at low temperatures all domain walls which appear as thermal fluctuations form closed loops.

If one considers an infinite straight domain wall and fixes the state (the values of φ_i) on one side of the wall, the state on the other side of the wall cannot be arbitrary and depends on the position and on the orientation of the wall [8,10]. If the wall is displaced by one lattice constant, the values of φ_i on the other side of the wall are changed by π.

The presence of a kink (of the minimal height) on a domain wall [Fig. 1(a)] produces a mismatch of π between the states which have to be obtained when crossing the left and the right parts of the wall. This discrepancy has to be taken care of by a fractional vortex with the topological charge $\pm 1/2$ located on the kink. The energy of such a simple kink is therefore logarithmically divergent. The kinks of the double (or, generally, even) height [Fig. 1(b)] do not introduce any mismatch, and their energy is finite.

Let us consider an infinite domain wall, introduced, for example, by an appropriate choice of boundary conditions. At low temperatures, it should contain a finite concentration of free double kinks, but all simple kinks have to form neutral pairs. Therefore, although the fluctuations of the domain wall diverge, the symmetry with respect to its shift by one lattice constant is broken.

With an increase of temperature, the phase transition in the one-dimensional logarithmic gas of simple kinks will lead to dissociation of neutral pairs and to the appearance of a finite concentration of free simple kinks [14]. As follows from the renormalization group analysis of Ref. [18], this takes place when the prefactor of the logarithmic interaction of simple kinks is equal to $2T$, that is, at

$$T_{\rm K} = \frac{\pi}{4}\,\Gamma(T_{\rm K})\,. \tag{3}$$

Here $\Gamma(T)$ is the helicity modulus, the macroscopic parameter describing the effective stiffness of the system with respect to continuous twist of φ. At zero temperature $\Gamma(0) = J/\sqrt{2}$, whereas the unbinding of integer vortices "in the bulk" takes place at [19]

$$T_{\rm V} = \frac{\pi}{2}\,\Gamma(T_{\rm V})\,, \tag{4}$$

that is, above $T_{\rm K}$. The numerical evidence for unbinding of kink pairs at $T_{\rm K} < T_{\rm V}$ has been obtained by Lee *et al.* [14], who, however, mistook this phase transition for the roughening transition of domain walls.

The phase transition associated with unbinding of pairs of simple kinks leads to a restoration of the symmetry between the odd and the even positions of the domain wall and also to the loss of the effective phase stiffness across the wall. Any attempt to create a phase gradient perpendicularly to the wall will be relaxed due to the motion of free simple kinks along the wall in different directions (in accordance with the sign of the topological charge) under the action of Magnus force. The situation is analogous to what happens in the bulk above $T_{\rm V}$, when the presence of free vortices prevents the creation of any stationary phase gradient (supercurrent). For $T < T_{\rm K}$, all simple kinks are bound in neutral pairs and their relative displacement requires a finite energy, which means that the phase stiffness across the wall remains finite.

Analogously, a phase gradient parallel to the wall will not penetrate on the other side of the wall. Instead there will appear a difference in concentration of simple kinks with positive and negative topological charges, which will compensate for the difference in phase gradients on both sides of the wall. Although the creation of such a difference in concentrations requires some energy, this energy is proportional to the length of the wall, whereas penetration of the phase gradient across the wall would require the additional energy which is proportional to the total area of the domain on the other side of the wall. The same happens on grain boundaries in crystals, where the difference in orientations is taken care of by a sequence of dislocations of the same sign.

Note that both mechanisms work only at length scales which are large in comparison with the inverse linear concentration of free simple kinks. Nonetheless, their existence implies that at large length scales the FF XY model can indeed be approximated by the XY-Ising model as proposed in Refs. [12,13]. Naturally, at $T < T_{\rm DW}$ such equivalence works only in a small vicinity of $T_{\rm DW}$, in which the correlation length, defined in terms of σ, is much larger than the typical distance between free simple kinks on a domain wall.

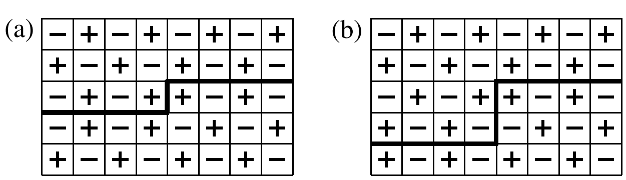

FIG. 1. A domain wall with (a) a simple kink and (b) a double kink. Plusses and minuses show the signs of chiralities.

The same conclusions are valid in the case of the antiferromagnetic XY model on a triangular lattice. The ground state of this model consists of three sublattices, the values of φ_i in which differ by $\pm 2\pi/3$, and also is characterized by the $U(1) \times Z_2$ degeneracy [3]. If the ground state on one side of a straight domain wall is fixed, the state on the other side of the wall can be obtained by a permutation of values of φ_i on any two sublattices and subsequent rotation of all variables by π [9].

The three available options correspond to three positions of the wall and differ from each other by global rotation by $\pm 2\pi/3$. Therefore, the simple kinks separating the straight parts of a domain wall have to behave as fractional vortices with topological charges $\pm 1/3$. Accordingly, the phase transition associated with kink pairs unbinding on an isolated infinite domain wall takes place at $T_K^\Delta = (\pi/9)\Gamma(T_K^\Delta)$, which is again below T_V. As in the case of a square lattice, this phase transition leads to the loss of phase coupling across a domain wall and makes the behavior of the system analogous to that of the XY-Ising model.

The helicity modulus Γ can be defined, in particular, through the response of a system to application of the specially chosen boundary conditions (see, for example, Ref. [20]). The important property of the XY-Ising model is that, as soon as there is at least one domain wall crossing the whole system, the variables φ at opposite boundaries are completely decoupled from each other, which means $\Gamma \equiv 0$. In the thermodynamic limit this takes place at any temperature higher than T_{DW}.

At $T < T_{DW}$ an externally imposed twist of φ in any typical configuration of s_i can be carried only by the largest (infinite) cluster formed by the sites with the same sign of s_i [note that the variable s_i of the XY-Ising model (2) should be associated with the staggered chirality of the FF XY model and not with the chirality itself]. All other clusters have finite size and therefore are insensitive to boundary conditions.

In two dimensions (in contrast to three), the point of the phase transition of the Ising model coincides with the percolation transition in the system of spin clusters [21], so the density of the infinite cluster decays on approaching T_{DW} from below as $\rho(T) \propto \xi_p^{-\Delta d}$. Here $\Delta d = 2 - \overline{d} = 5/96$ [22] is the deviation of the fractal dimension $\overline{d}$ of the infinite cluster (at $T = T_{DW}$) from its Euclidean dimension and $\xi_p(T) \propto (T_{DW} - T)^{-\nu}$ is the percolation length, the temperature dependence of which in the Ising model is described by the same exponent $\nu = 1$ [23] as that of the correlation length ξ.

Therefore the bare (i.e., not reduced by the fluctuations of φ) helicity modulus $\Gamma_0(T)$ on approaching T_{DW} has to decrease algebraically: $\Gamma_0(T) \propto (T_{DW} - T)^t$, at least as fast as $\rho(T)$ (actually much faster), which can be shown with the help of the variational calculation. The vortex pair dissociation takes place as soon as the (renormalized) value of Γ is reduced to $(2/\pi)T$, that is, below T_{DW}. For $T_{DW} \ll T_V^{(0)}$ [where $T_V^{(0)} \approx (\pi/2)\Gamma(0)$ is the naive estimate for T_V], one therefore can expect $T_{DW} - T_V \propto [T_{DW}/T_V^{(0)}]^{1/t}$. The two transitions can happen simultaneously only if they occur as the first-order phase transition with a larger than universal jump in Γ.

According to our results, the analogous behavior can be expected in the FF XY models. However, in that case the dependence of $T_{DW} - T_V$ on T_{DW} will be more complicated, since the effective reduction to the XY-Ising model is developed only at the length scales which are large in comparison with typical distance between free simple kinks. The idea that $\Gamma_0(T)$ is strongly suppressed on approaching T_{DW} is supported by a comparison of the results of numerical simulations of the same system at zero and full frustration [7], which shows that in the latter case the drop of Γ with an increase of temperature for the same size of the system is more sharp.

In conclusion, until now the use of the XY-Ising model for the description of the properties of the FF XY model on a square lattice [13,24] could be considered a rather arbitrary procedure. Since application of the Hubbard-Stratanovich transformation [11] to the FF XY model on a triangular lattice is known to produce a coarse-grained Hamiltonian [12] with a wrong symmetry of the ground state [$U(1) \times Z_3$ instead of $U(1) \times Z_2$], one always could doubt if the application of the same transformation on a square lattice does not lead to the loss of some important properties of the original model.

An argument in favor of such an approach has been put forward by Knops *et al.* [20], who have shown, with the help of the numerical transfer matrix diagonalization, that at $T = T_{DW}$ the free energy of the 19-vertex version of the FF XY model with increasing the system size becomes insensitive to the boundary conditions inducing the twist of φ. The authors of Ref. [20] have interpreted this as evidence for irrelevance at criticality of the coupling of φ across a domain wall. The same observation could be alternatively interpreted as evidence for $T_V < T_{DW}$.

In the present Letter we have demonstrated that in the FF XY models on square and triangular lattices the loss of the phase coupling across domain walls is achieved already at temperatures below T_V due to the presence on domain walls of free simple kinks. We also have shown that the dissociation of vortex pairs has to take place at $T_V < T_{DW}$, because, on approaching T_{DW} from below, the part of the system which reacts to external twist becomes more and more dilute [25]. This makes the scenario of a single phase transition with a novel critical behavior [9,26] impossible, at least for $T > T_K$.

These conclusions are not dependent on the particular form of the interactions in the system (as soon as the degeneracy of the ground state remains the same), and are applicable, for example, also when the interaction of further neighbors is taken into account [27]. They are in agreement with the results of the most recent numerical simulations of the FF XY models on square [28,29] and triangular

[30] lattices, as well as of the equivalent (half-integer) Coulomb gas [31] and of the solid-on-solid (SOS)–Ising model [32] which is (partially) dual to the XY-Ising model.

Recently Lee *et al.* [32] have demonstrated that the generalized XY-Ising model is dual to the SOS-Ising model introduced by den Nijs [15] for the coarse-grained description of the interplay between roughening and missing row reconstruction on a surface of a crystal with a simple cubic lattice. The proposed phase diagram of this model can be found in Fig. 3 of Ref. [16]. For the case of $\Delta = 0$ (which corresponds to the XY-Ising model with a complete absence of phase coupling across domain walls), it contains two regions, one (at $R < 0$) with separated and the other (at $R > 0$) with coinciding phase transitions. Our analysis, as well as the results of the numerical simulations of Ref. [32], implies that the two transitions should be separated for both signs of R.

It seems worthwhile to mention that the conclusion on a larger than universal value of $\Gamma(T_V)$ in the FF XY models [29–31] has been obtained with the help of the Weber-Minnhagen (WM) scaling analysis [33], which is based on the same renormalization group equations [6] as the universal prediction (4) and, accordingly, does not even allow for a possibility of a nonuniversal value of $\Gamma(T_V)$. The results of Refs. [29–31] therefore should be interpreted as evidence for deviation from the WM scaling. The reasons for such a deviation can be easily understood. It follows from our analysis that, even when the presence of vortex pairs (the only factor taken into account in the framework of the WM analysis) is neglected, Γ in the vicinity of T_{DW} has to be strongly scale dependent, because the effects related to suppression of the effective stiffness across domain walls develop only with the increase of scale. Thus it is important not to confuse the two mechanisms for suppression of Γ. The method for plotting the data, which allows for checking in what interval of length scales the WM scaling really holds, has been recently suggested in Ref. [27].

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[1] P. Martinoli and Ch. Leemann, J. Low Temp. Phys. **118**, 699 (2000), and references therein.
[2] J. Villain, J. Phys. C **10**, 1717 (1977).
[3] D. H. Lee, R. G. Caflisch, J. D. Joannopoulos, and F. Y. Wu, Phys. Rev. B **29**, 2680 (1984); S. Miyashita and J. Shiba, J. Phys. Soc. Jpn. **53**, 1145 (1984).
[4] V. L. Berezinskii, Zh. Eksp. Teor. Fiz. **61**, 1144 (1971) [Sov. Phys. JETP **34**, 610 (1972)].
[5] J. M. Kosterlitz and D. J. Thouless, J. Phys. C **5**, L124 (1972); **6**, 1181 (1973).
[6] J. M. Kosterlitz, J. Phys. C **7**, 1046 (1974).
[7] S. Teitel and C. Jayaprakash, Phys. Rev. B **27**, 598 (1983).
[8] T. C. Halsey, J. Phys. C **18**, 2437 (1985).
[9] S. E. Korshunov and G. V. Uimin, J. Stat. Phys. **43**, 1 (1986).
[10] S. E. Korshunov, J. Stat. Phys. **43**, 17 (1986).
[11] R. L. Stratanovich, Dokl. Akad. Nauk SSSR **115**, 1097 (1957) [Sov. Phys. Dokl. **2**, 416 (1958)]; J. Hubbard, Phys. Rev. Lett. **3**, 77 (1959).
[12] M. Y. Choi and S. Doniach, Phys. Rev. B **31**, 4516 (1985); M. Yosefin and E. Domany, Phys. Rev. B **32**, 1778 (1985).
[13] E. Granato, J. M. Kosterlitz, J. Lee, and M. P. Nightingale, Phys. Rev. Lett. **66**, 1090 (1991); J. Lee, E. Granato, and J. M. Kosterlitz, Phys. Rev. B **44**, 4819 (1991).
[14] S. J. Lee, J.-R. Lee, and B. Kim, Phys. Rev. E **51**, R4 (1995); J.-R. Lee, S. J. Lee, B. Kim, and I. Chang, Phys. Rev. Lett. **79**, 2172 (1997).
[15] M. den Nijs, Phys. Rev. B **46**, 10 386 (1992).
[16] D. Davidson and M. den Nijs, Phys. Rev. E **55**, 1331 (1997).
[17] S. E. Korshunov, Phys. Rev. B **63**, 134503 (2001).
[18] S. A. Bulgadaev, Phys. Lett. **86A**, 213 (1981); Teor. Mat. Fiz. **51**, 424 (1982) [Theor. Math. Phys. **51**, 593 (1982)].
[19] D. R. Nelson and J. M. Kosterlitz, Phys. Rev. Lett. **39**, 1201 (1977).
[20] Y. M. M. Knops, B. Nienhuis, H. J. F. Knops, and H. W. J. Blöte, Phys. Rev. B **50**, 1061 (1994).
[21] A. Coniglio, C. R. Nappi, F. Peruggi, and L. Russo, J. Phys. A **10**, 205 (1977).
[22] A. L. Stella and C. Vanderzande, Phys. Rev. Lett. **62**, 1067 (1989); C. Vanderzande and A. L. Stella, J. Phys. A **22**, L445 (1989).
[23] W. Klein, H. E. Stanley, P. J. Reynolds, and A. Coniglio, Phys. Rev. Lett. **41**, 1145 (1978).
[24] E. Granato, J. Phys. C **20**, L215 (1987); M. P. Nightingale, E. Granato, and J. M. Kosterlitz, Phys. Rev. B **52**, 7402 (1995).
[25] The conjecture that $\Gamma(T)$ vanishes at $T = T_{DW}$, which leads to $T_V < T_{DW}$, was first made by Vik. S. Dotsenko and G. V. Uimin, Pis'ma Zh. Eksp. Teor. Fiz. **40**, 236 (1984) [JETP Lett. **40**, 1009 (1984)]; J. Phys. C **18**, 5019 (1985).
[26] J. Lee, J. M. Kosterlitz, and E. Granato, Phys. Rev. B **43**, 11 531 (1991).
[27] G. Franzese, V. Cataudella, S. E. Korshunov, and R. Fazio, Phys. Rev. B **62**, R9287 (2000).
[28] P. Olsson, Phys. Rev. Lett. **75**, 2758 (1995); **77**, 4850 (1996); Phys. Rev. B **55**, 3585 (1997).
[29] S. Lee and K.-C. Lee, Phys. Rev. B **49**, 15 184 (1994).
[30] S. Lee and K.-C. Lee, Phys. Rev. B **57**, 8472 (1998).
[31] J.-R. Lee, Phys. Rev. B **49**, 3317 (1994).
[32] S. Lee, K.-C. Lee, and J. M. Kosterlitz, Phys. Rev. B **56**, 340 (1997).
[33] H. Weber and P. Minnhagen, Phys. Rev. B **37**, 5986 (1988).