

Fluctuations and Vortex-Pattern Ordering in the Fully Frustrated XY Model on a Honeycomb Lattice

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The accidental degeneracy of various ground states of a fully frustrated XY model with a honeycomb lattice is shown to survive even when the free energy of the harmonic fluctuations is taken into account. The reason for that consists in the existence of a hidden gauge symmetry between the Hamiltonians describing the harmonic fluctuations in all these ground states. A particular vortex pattern is selected only when anharmonic fluctuations are taken into account. However, the observation of vortex ordering requires relatively large system size $L \gg L_c \approx 10^5$.

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A fully frustrated XY model can be defined by the Hamiltonian

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

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 $\sum A_{ij} = \pi \pmod{2\pi}$ (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 [1] in relation with experiments on Josephson junction arrays [2], in which φ_i can be associated with the phase of the superconducting order parameter on the i -th 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. Planar magnets with odd number of antiferromagnetic bonds per plaquette [3] are also described by fully frustrated XY models. Recently, the active interest in fully frustrated Josephson arrays has been related to their possible application for creation of topologically protected quantum bits [4].

The ground states of the fully frustrated XY models are characterized by the combination of the continuous $U(1)$ degeneracy (related with the possibility of the simultaneous rotation of all phases) and discrete degeneracy related with the distribution of positive and negative half-vortices between the lattice plaquettes. Since vortices of the same sign repel each other, the energy is minimized when the vorticities of the neighboring plaquettes are of the opposite sign. In the case of a square

lattice this requirement is fulfilled for all pairs of neighboring plaquettes when the vortices of different signs form a regular checkerboard pattern [3]. Analogous patterns, in which the vorticities of the neighboring plaquettes are always of the opposite sign, can be constructed in the case of a triangular lattice [5].

In the case of a honeycomb lattice it is impossible to construct a configuration in which the vorticities are of the opposite sign for all pairs of neighboring plaquettes. As a consequence, the discrete degeneracy of the ground state turns out to be much more developed [6,7], and can be described in terms of formation of zero-energy domain walls in parallel to each other [8], the residual entropy of the system being proportional to its linear size. Quite remarkably, the comparison of the free energies of weak fluctuations in two different periodic ground states shows that in harmonic approximation they are exactly equal to each other [8], although the spectra of fluctuations $\lambda(\mathbf{k})$ in these states are essentially different: for example, for small momenta \mathbf{k} they are characterized by different values of (anisotropic) helicity moduli.

In the present Letter we demonstrate that this absence of degeneracy lifting is not a simple coincidence, but a consequence of a hidden gauge symmetry between the Hamiltonians of harmonic fluctuations in different ground states, and extends itself to all states formed by some sequence of parallel zero-energy domain walls. Therefore, the inclusion of harmonic fluctuations will not lead to removal of the accidental degeneracy even if instead of considering thermodynamic fluctuations, one calculates the free energy of quantum fluctuations at arbitrary (or zero) temperature.

This gauge symmetry is broken when anharmonicities are taken into account. We have compared the leading anharmonic contributions to the free energies corresponding to different ground states and have found which of these states is selected at low temperatures. However,

the difference between their free energies turned out to contain extremely small numerical coefficients. As a consequence, the observation of vortex ordering is possible only in relatively large systems (whose size $L \gg L_c \approx 10^5$).

We believe that the discovery of these new features (some of which are completely unexpected) makes our results of interest not only in relation with Josephson junction array physics, but also in the more general context of two-dimensional statistical mechanics.

Figure 1(a) shows a structure of the simplest ground state of the fully frustrated XY model with a honeycomb lattice. Each arrow corresponds to $\theta_{ij} = \varphi_j - \varphi_i - A_{ij} = \pi/4$, whereas on the bonds without arrows, $\theta_{ij} = 0$. In this state the plaquettes with positive and negative vorticities form straight stripes, so in the following we shall call it a striped state.

A striped state allows for formation of domain walls (separating two different realizations of such state) which cost no energy [8]. An example of such zero-energy domain wall is shown in Fig. 1(b). An arbitrary number of zero-energy domain walls separated by arbitrary distances can be introduced into the system in parallel to each other [8].

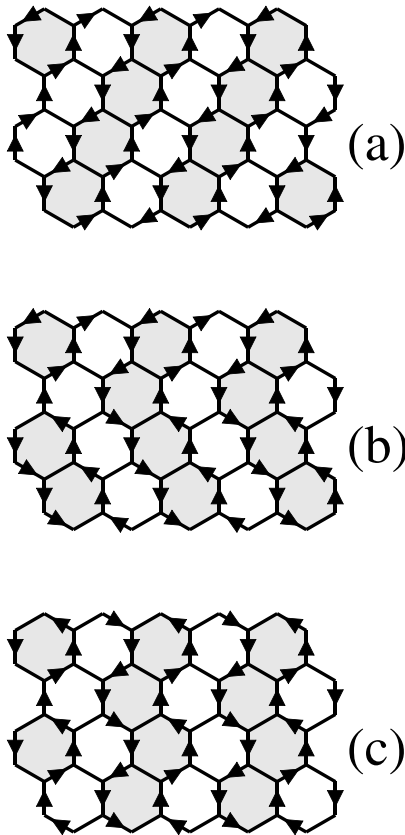


FIG. 1. Three different ground states of a fully frustrated XY model with a honeycomb lattice: (a) striped state, (b) zero-energy domain wall, and (c) zig-zag state. Directed arrows (or their absence) correspond to $\theta_{ij} = \pi/4$ ($\theta_{ij} = 0$). Lattice plaquettes with positive vorticities are shaded.

If such domain walls are created at every possible position, another periodic ground state is obtained, which is shown in Fig. 1(c). In accordance with the shape of the lines formed by the plaquettes with positive and negative vorticities in this state we shall call it a zig-zag state. Alternatively, one can describe all other ground states as obtained by the introduction of zero-energy domain walls on the background of a zig-zag state.

If all sites of a honeycomb lattice are numbered by pairs of integers (n, m) as shown in Fig. 2, the Hamiltonian describing the harmonic fluctuations in the striped state of Fig. 1(a) can be written as:

$$H_a^{(2)} = \frac{1}{2} \sum_n \sum_{m=n(\text{mod}2)} [J_1(u_{n,m} - v_{n,m-1})^2 + J_2(u_{n,m} - v_{n+1,m})^2 + J_3(u_{n,m} - v_{n-1,m})^2], \quad (2)$$

where $J_1 = J_2 = J \cos(\pi/4)$, $J_3 = J$, whereas $u_{n,m}$ and $v_{n,m}$ are the deviations of the variables φ from their equilibrium values on two triangular sublattices forming a honeycomb lattice.

If one assumes the presence of periodic boundary conditions in the horizontal direction and open boundary conditions in the perpendicular (vertical) direction, the introduction of plane waves with respect to the variable n allows to rewrite Eq. (2) as:

$$H_a^{(2)} = \frac{1}{2} \int \frac{dq}{2\pi} \sum_m \{J_S[|u_m(q)|^2 + |v_m(q)|^2] - J_1[u_{m+1}(q)v_m^*(q) + \text{c.c.}] - [K(q)u_m(q)v_m^*(q) + \text{c.c.}]\}, \quad (3)$$

where $J_S = J_1 + J_2 + J_3$ and $K(q) = J_2 \exp(-iq) + J_3 \exp(iq)$. A trivial gauge transformation:

$$\begin{pmatrix} u_{m+1}(q) \\ v_m(q) \end{pmatrix} \Rightarrow \exp[i\alpha(q)m] \times \begin{pmatrix} \tilde{u}_{m+1}(q) \\ \tilde{v}_m(q) \end{pmatrix}, \quad (4)$$

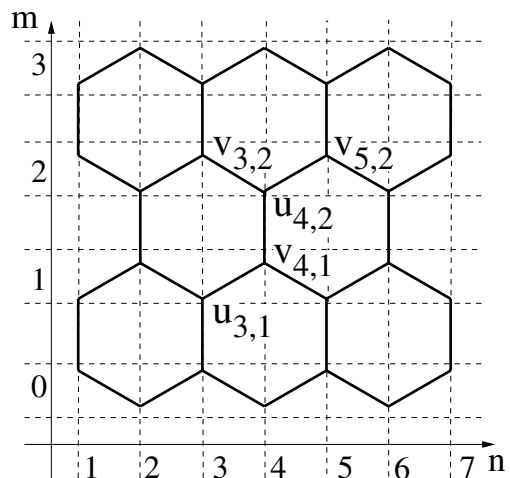


FIG. 2. The numbering of a honeycomb lattice sites by a pair of integers (n, m) used when writing Eq. (2).

where $\alpha(q) = \arg[K(q)]$, allows then to replace Eq. (3) by the analogous expression with $K_0(q) \equiv |K(q)|$ substituted for $K(q)$.

Note that in the chosen mixed representation, the only modification of the Hamiltonian which appears when an arbitrary sequence of horizontal domain walls is introduced consists in replacement of $K(q)$ by $K^*(q)$ for some values of m . It is rather evident that the gauge transformation analogous to Eq. (4) (in which $\alpha(q)m$ should be replaced by $\alpha(q)\sum_{m' < m} s_{m'}$, where variable $s_m = \pm 1$ describes the choice between the two options existing for the continuation of a ground state at each m) allows to transform any such Hamiltonian to the same form (with $K(q)$ replaced everywhere by $K_0(q)$).

This means that for the boundary conditions described above, the whole set of eigenvalues will be exactly the same for all Hamiltonians obtained by the introduction of an arbitrary sequence of horizontal domain walls (even for a finite sample). Accordingly, the free energy of the harmonic fluctuations will be exactly the same, and cannot be the source for the selection of a particular ground state.

Clearly, the free energy of harmonic fluctuations also remains degenerate when one considers a quantum generalization of the same model with the diagonal mass term, which in terms of a Josephson junction array, corresponds to taking into account the self-capacitance of each superconducting island [9]. In order to include into consideration the mutual capacitances of neighboring islands (that is, the capacitances of the junctions), one has to apply the same approach (construction of the gauge transformation which makes all the coefficients real) not to the harmonic part of the Hamiltonian, but to the frequency dependent Fourier transform of the harmonic contribution to Euclidean Lagrangian, which also turns out to be possible. That means that in the quantum version of the model, the accidental degeneracy survives (at the harmonic level) for arbitrary relation between the self-capacitance of an island and the capacitance of a junction.

If one assumes now periodic boundary conditions in the vertical direction (instead of open boundaries), the degeneracy of the free energy associated with harmonic fluctuations (quantum or thermodynamic) will be manifested only in the thermodynamic limit.

The accidental degeneracy of different ground states is removed when anharmonicities are taken into account. The leading contribution to the free energy induced by anharmonic fluctuations, F_{anh} , is given by the sum of two terms, which in the classical limit can be written as $F^{(3)} = -\langle [H^{(3)}]^2 \rangle / 2T$ and $F^{(4)} = \langle H^{(4)} \rangle$, where $H^{(3)}$ and $H^{(4)}$ are, respectively, the third- and the fourth-order corrections to the harmonic part of the Hamiltonian.

Since each term in $F^{(4)}$ depends only on local phase difference on a particular bond, it can be proven with the help of the hidden gauge symmetry discussed above that in the considered system, $F^{(4)}$ is the same for all ground

states. However, this property does not extend itself to $F^{(3)}$, which depends also on more distant correlations.

Comparison of the expressions for $F^{(3)}$ in the two different periodic ground states shows that the main contribution to $\delta F = F_{\text{zig-zag}}^{(3)} - F_{\text{str}}^{(3)}$ (normalized per single hexagon) can be written as

$$\delta F = -6(G_s^3 + G_z^3)J_*^2/T, \quad (5)$$

where $J_* = J \sin(\pi/4)/6$, whereas

$$G_s = \langle (u_{n,m} - v_{n+1,m})(u_{n+1,m-1} - v_{n+2,m-1}) \rangle \quad (6)$$

and

$$G_z = \langle (u_{n,m} - v_{n+1,m})(u_{n+1,m-1} - v_{n,m-1}) \rangle \quad (7)$$

are two correlation functions (for the bonds with $|\theta_{ij}| = \pi/4$), calculated with the help of the harmonic Hamiltonian in striped and zig-zag states, respectively.

Numerical calculation of the corresponding integrals over Brillouin zone gives $G_s \approx 0.1559 T/J$ and $G_z \approx -0.1686 T/J$, which after substitution in Eq. (5) leads to $\delta F \approx \gamma T^2/J$, where $\gamma \approx 0.8 \times 10^{-4}$. Addition to Eq. (5) of the terms associated with more distant pairs of bonds leads only to a slight reduction of the numerical coefficient to $\gamma \approx 0.7 \times 10^{-4}$.

Thus we have demonstrated that $\delta F \propto T^2$, as in the case of the antiferromagnetic XY model with a kagomé lattice [10,11]. In situations, when a so-called “order-from-disorder” mechanism [12] works already at the harmonic level, the free energy difference between the accidentally degenerate ground states of frustrated XY models is proportional to the first power of T [13–16].

The fluctuation induced free energy (per unit length) of a zero-energy domain wall on the background of a striped state [see Fig. 1(b)] is also given by δF . It has been shown in Ref. [16] that in the frustrated XY-models with accidental degeneracy which manifests itself in the possibility of formation of zero-energy domain walls, the temperature of the phase transition associated with vortex pattern disordering (that is, with the proliferation of such walls) can be estimated as

$$T_c \approx E_K / \ln[T_c / \delta F(T_c)], \quad (8)$$

where $E_K \sim J$ is the energy of a kink on a domain wall and $\delta F(T)$ is the fluctuation induced free energy of a domain wall (per unit length). For $\gamma \sim 10^{-4}$ the logarithmical factor in Eq. (8) is close to 12, which means that the extreme smallness of $\delta F(T)$ in the considered problem leads to the reduction of T_c (in comparison with E_K) by 1 order of magnitude.

However, the extreme smallness of $\delta F(T)$ manifests itself much more strongly in the relative prominence of the finite size effects. For $\delta F(T) \approx \gamma T^2/J$ the (normalized) probability to have a domain wall crossing a finite system of the width L can be estimated as $\exp[-(\gamma T/J)L]$ and is much smaller than 1 only for $L \gg L_c = J/\gamma T$, which in our case gives $L_c \approx 10^5$.

This means that although anharmonic fluctuations in the fully frustrated XY model with a honeycomb lattice lead to the existence of a thermodynamic phase transition (related with vortex pattern ordering) at not too small temperature $T_c \sim 10^{-1}J$, the sizes of Josephson junction arrays available experimentally, as well as the sizes of the systems which can be simulated in numerical experiments, are currently not sufficient for observation of this ordering.

To conclude, in the present Letter we have demonstrated that the fully frustrated XY model with a honeycomb lattice is the first example of a statistical model in which the accidental degeneracy of different ground states is not removed by the free energy of harmonic fluctuations (neither in the classical nor in the quantum version of the model), although in different states these fluctuations are described by different Hamiltonians. The responsibility for that can be traced to a hidden gauge symmetry, which manifests itself when these Hamiltonians are rewritten in terms of the mixed representation.

We also have shown that accidental degeneracy is removed by the free energy of anharmonic fluctuations, which leads to the selection of a striped state of the type shown in Fig. 1(a). The state with analogous vortex configuration is selected as well in a fully frustrated superconducting wire network with honeycomb geometry (in the vicinity of the phase transition), but for entirely different reasons related with the possibility of the order parameter modulation [17].

However, the estimates based on numerical calculation of the anharmonicity induced domain wall free energy show that the system size ($L \gg 10^5$), which is required for the observation of vortex ordering in the fully frustrated XY model on a honeycomb lattice is much larger than those which are typical for experiments or numerical simulations, which makes the observation of such an ordering rather problematic. It should be emphasized that although the considered model with a honeycomb lattice has been the subject of Monte Carlo simulations of Shih and Stroud [7,18], these authors have not analyzed the structure of vortex pattern. In the experimental situation, the magnetic interactions of currents in a Josephson junction array will be of greater importance for the stabilization of a particular vortex pattern than the anharmonic fluctuations.

The ideas developed here may also be extended to other geometries under current investigations. One of the most intriguing systems in this respect is the fully frustrated XY model on a dice lattice, which exhibits a similar degeneracy between its classical ground states [19], and has been the subject of recent experiments [20] and numerical simulations [21]. In particular, one of the main reasons for the absence of vortex ordering in magnetic decoration experiments of Ref. [20], as well as in numerical simulations of Ref. [21] is very likely to be a not sufficient system size.

The conclusion on relative prominence of finite size effects (leading to the destruction of long range order) in situations when the stability of a vortex pattern is induced only by anharmonic fluctuations is applicable to even wider classes of models. Their number includes the anti-ferromagnetic XY model with a *kagomé* lattice [10,11,22], in which, in the thermodynamic limit, the anharmonic corrections to free energy lead to the stabilization of so-called $\sqrt{3} \times \sqrt{3}$ state at $T < T_c \sim 10^{-4}J$ [11]. However, the estimates analogous to those performed above allow one to conclude that the observation of such an ordering is possible only when $L \gg L_c \sim 10^7$, that is, only in truly macroscopic systems. In numerical simulations of Ref. [22], this condition definitely was not satisfied.

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